Flame Studies of Jet Fuels and Surrogate-Related Neat Hydrocarbons

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MULTI AGENCY COORDINATION COMMITTEE
FOR COMBUSTION RESEARCH (MACCCR)
5th Annual FUELS RESEARCH REVIEW

September 17-20, 2012
Combustion Research Facility (CRF)
Sandia National Laboratory

AFOSR Grant: FA9550-11-1-0217 (AFRL Energy IPT)
Period of performance: 9/1/11 – 8/31/14

Contract Monitor: Dr. Chiping Li

General Objectives

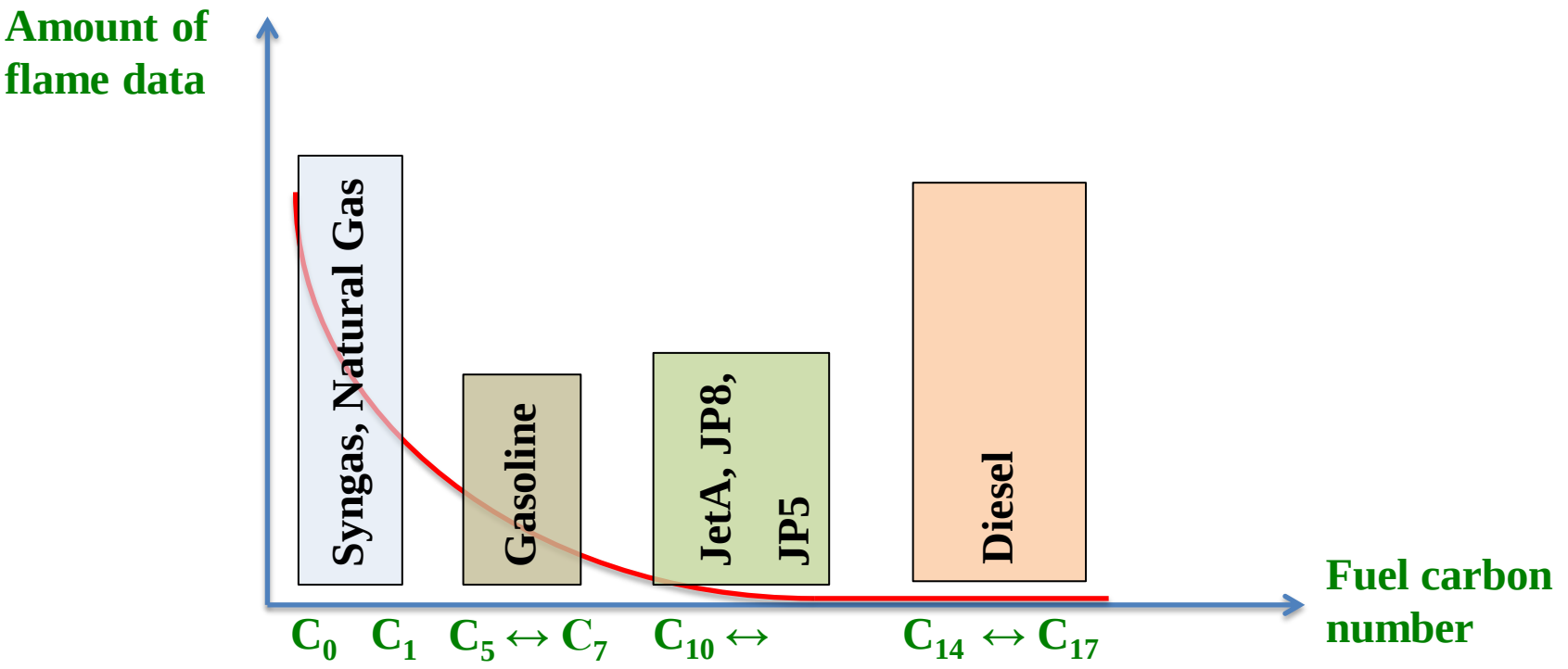
- **To derive fundamental understanding of the combustion behavior under conditions of relevance to high-speed air-breathing propulsion in flames of:**
  - **Conventional and alternative jet fuels**
  - **Neat heavy hydrocarbons that are candidate components of fuel surrogate formulations**

- **To contribute towards the development of attendant chemical kinetic models by identifying the rate controlling mechanisms under relevant flame conditions.**

- **To obtain physical and chemical understanding that could contribute to existing turbulent combustion knowledge in the context of large molecular weight fuels.**

Background (1)

- Large MW fuels are characterized by very low vapor pressure.
- Establishing flames with pre-vaporized fuel presents a major challenge – conflicting requirements of achieving higher vapor pressure and fuel decomposition through fuel pre-heating.
- Flame data are scarce for > C_{12} fuels, even at 1 atm:



Background (2)

- **Flow conditions in air-breathing propulsion engines are highly turbulent.**

- **Over the years, turbulent combustion research has provided extensive data-bases either from experiments or from simulations.**

- **However, the vast majority of information has been derived from studies in which:**
  - ✧ **small MW fuels, e.g. H_2 or CH_4, have been used, and/or**
  - ✧ **the chemical aspects of the fuel oxidation are suppressed to a bare minimum (e.g., 1-step kinetics) in order to augment the emphasis on turbulence**

Background (3)

- **Compared to H_2 and CH_4, heavy fuels have vastly different diffusive and chemical properties:**
  - **Diffusive properties can affect flame stability and response to turbulence**
  - **Heavy fuels tend to decompose easily, and what ends up "feeding" the flames may not be necessarily the parent molecule(s)**

- **Suppressing the details of fuel oxidation/pyrolysis of realistic heavy fuels may be questionable in predicting, for example:**
  - **Auto-ignition**
  - **Local extinction followed by re-ignition**
  - **Global extinction (blow-off)**
  - **The appropriate "laminar flame speed" needed to scale the "turbulent flame speed"**

Parameter Space

- **Fuels:**
  - JP-8 (petroleum-derived, synthetic, bio-derived, coal-derived)
  - $C_{5\text{-}12}$ *n*-alkanes (emphasis on *n*-dodecane)
  - $C_{5\text{-}12}$ *iso*-alkanes (emphasis on *2,7*-dimethyloctane)
  - $C_{7\text{-}12}$ *cyclo*-alkanes (emphasis on *n*-butylcyclohexane)
  - $C_{7\text{-}12}$ aromatics (emphasis on *n*-propylbenzene)
  - Selected binary and tertiary fuel mixtures
- **Thermodynamic pressure:**
  - $P = 1$ atm; "foundation" data
  - $P = 0.3 – 0.5$ atm; data relevant to high altitude relight
  - $P > 1$ atm; rather challenging for pre-vaporized fuels and alternative approaches will be considered
- **Unburned reactant temperature:**
  - $300\ \text{K} \leq T_u < 600\ \text{K}$; at ~ 600 K fuel decomposition initiates
- **Combustion phenomena:**
  - Flame response to highly intense turbulence
  - Flame propagation (under laminar and turbulent conditions)
  - Flame extinction/ignition (under laminar and turbulent conditions)

Summary of Results – Laminar Flames

- **Experimental and modeling investigations of flame propagation, extinction, and ignition under "standard" laminar conditions of P = 1 atm and elevated unburned mixture temperatures for the following fuels:**

- **jet fuels**
  - JP-7
  - JP-8
  - S-8
  - Shell-GTL
  - R-8

- ***n*-alkanes**
  - *n*-pentane
  - *n*-hexane
  - *n*-heptane
  - *n*-octane
  - *n*-nonane
  - *n*-decane
  - *n*-dodecane

- ***iso*-alkanes**
  - *2*-methylpentane
  - *3*-methylpentane
  - *2,5*-dimethylhexane
  - *2,2,4*-trimethylpentane (*iso*-octane)
  - *2,7*-dimethyloctane

- ***cyclo*-alkanes**
  - cyclohexane (CHX)
  - methyl-CHX
  - ethyl-CHX
  - *n*-propyl-CHX
  - *n*-butyl-CHX

- **aromatics**
  - benzene
  - toluene
  - *o*-xylene
  - *m*-xylene
  - *p*-xylene
  - *n*-propylbenzene
  - *1,2,4*-trimethylbenzene
  - *1,3,5*-trimethylbenzene

- **cyclopentadiene**
  - first flame data ever reported

Key Findings (1)

- **$C_{5\text{-}12}$ *n*-alkanes:**
  - **Due to fast fuel decomposition, C_0-C_4 kinetics control flame ignition, propagation, and extinction**

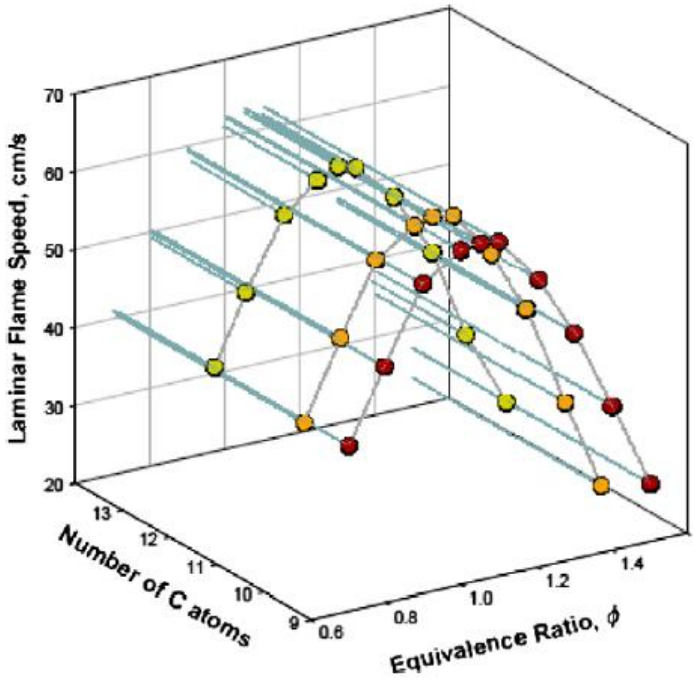


Fig. 11. Comparison of experimentally determined S_u^o's of mixtures of air with n-C_9H_{20}, n-$C_{10}H_{22}$, and n-$C_{12}H_{26}$ at T_u = 403 K.

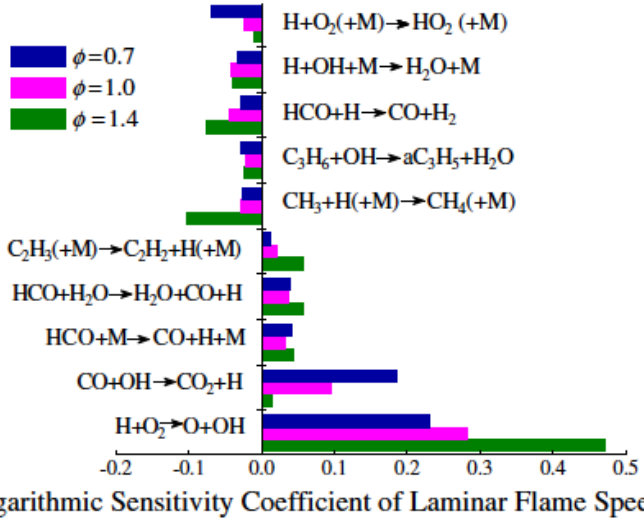


Fig. 6. Ranked logarithmic sensitivity coefficients of S_u^o on reaction rate coefficients, computed for n-$C_{12}H_{26}$/air mixtures at various ϕ's and T_u = 403 K.

Key Findings (2)

- ***Cyclo*-alkanes:**
  - **Flames of mono-alkylated cyclohexane compounds were found to have similar laminar flame speeds, from methylcyclohexane to *n*-butylcyclohexane, suggesting that the different alkyl groups have a secondary effect on flame propagation**
  - **C_0-C_4 kinetics control flame ignition and propagation**

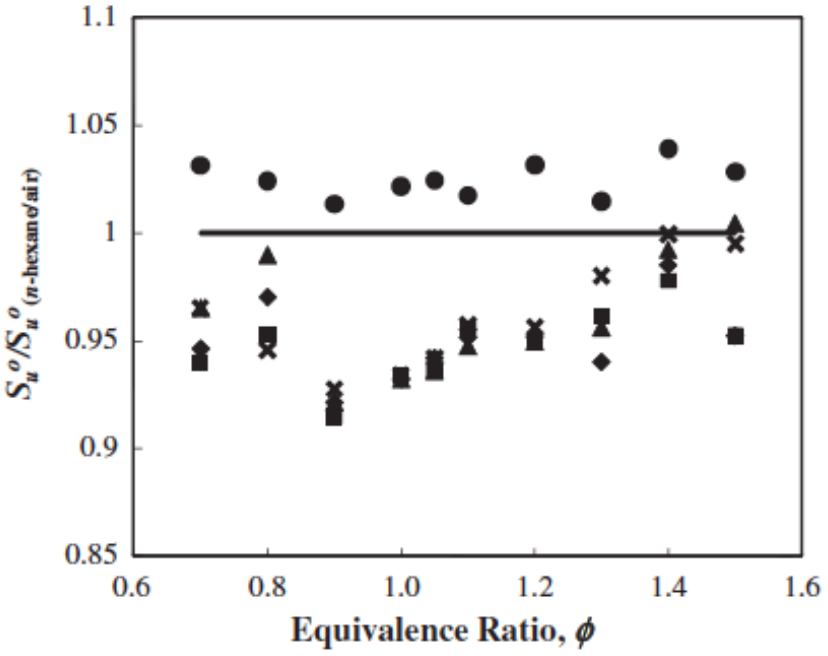


Fig. 6. Comparison of experimentally determined S_u^o's of (●) cyclohexane/air, (♦) methylcyclohexane/air, (■) ethylcyclohexane/air, (×) *n*-propylcyclohexane/air, and (▲) *n*-butylcyclohexane/air flames relative to those of (▬) *n*-hexane/air flames at $T_u = 353$ K.

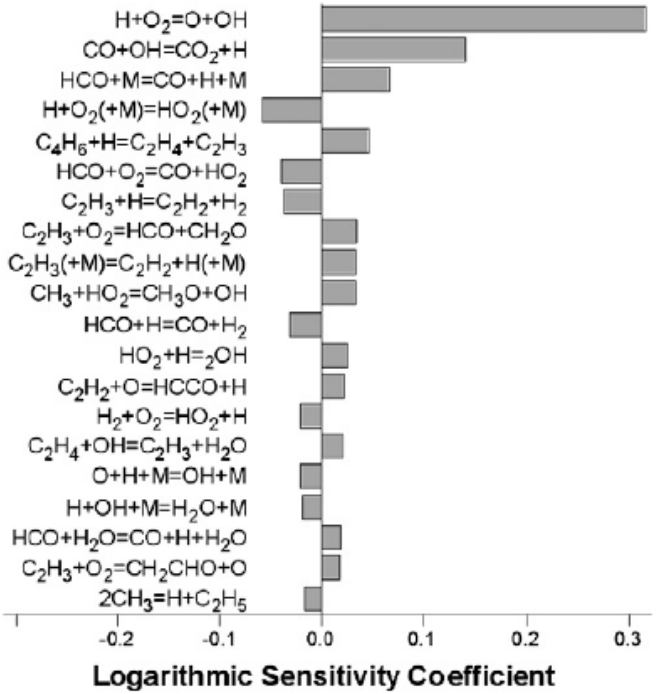


Fig. 3. Ranked logarithmic sensitivity coefficients of S_u^o with respect to reaction rate coefficients computed using Model I (JetSurF 1.1) for cyclohexane/air flames at $T_u = 353$ K and $p = 1$ atm.

Key Findings (3)

- ***Iso*-alkanes:**
  - **The extent of fuel branching was found to affect flame propagation and ignition**
  - **In addition to C_0-C_4 kinetics, fuel kinetics affect *moderately* flame ignition and propagation**

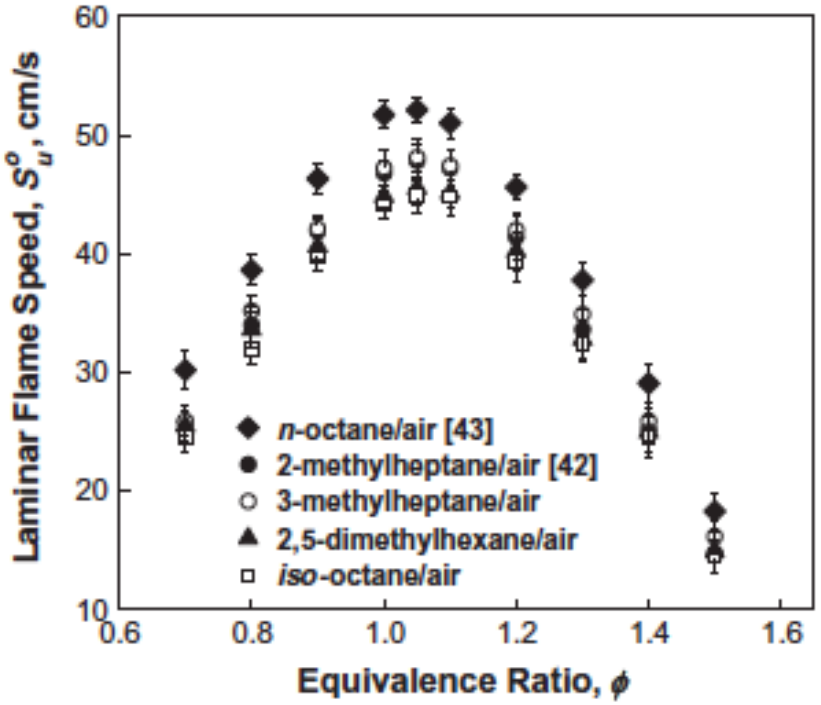


Fig. 3. Experimentally determined S_u^o's of *n*-octane/air [43], 2-methylheptane/air [42], 3-methylheptane/air, 2,5-dimethylhexane/air, and *iso*-octane/air mixtures at T_u = 353 K and p = 1 atm. The error bars represent 2σ uncertainty.

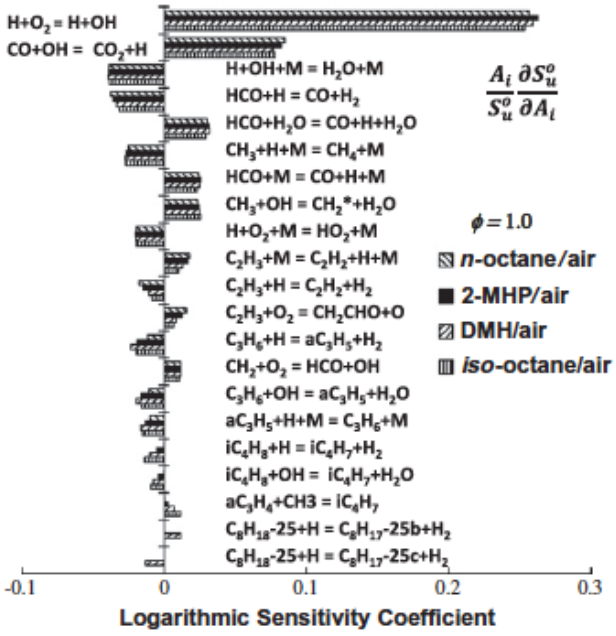


Fig. 12. Comparison of ranked logarithmic sensitivity coefficients of S_u^o on reaction rate coefficients, computed with Model II for stoichiometric *n*-octane/air, 2-MHP/air, DMH/air, and *iso*-octane/air mixtures at T_u = 353 K and p = 1 atm, in which DMH is denoted as C_8H_{18}-25, and C_8H_{17}-25b and C_8H_{17}-25c represent 2,5-dimethyl-2-hexyl and 2,5-dimethyl-3-hexyl radical separately.

Key Findings (4)

- **Aromatics and cyclopentadiene:**
  - **The propagation and extinction of benzene and alkylated benzene flames depend critically on the aromatic fuel structure and overall reactivity is reduced with the extent of methylation of benzene**
  - **In addition to C_0-C_4 kinetics, fuel kinetics are rate-controlling affecting thus *notably* flame propagation and extinction**

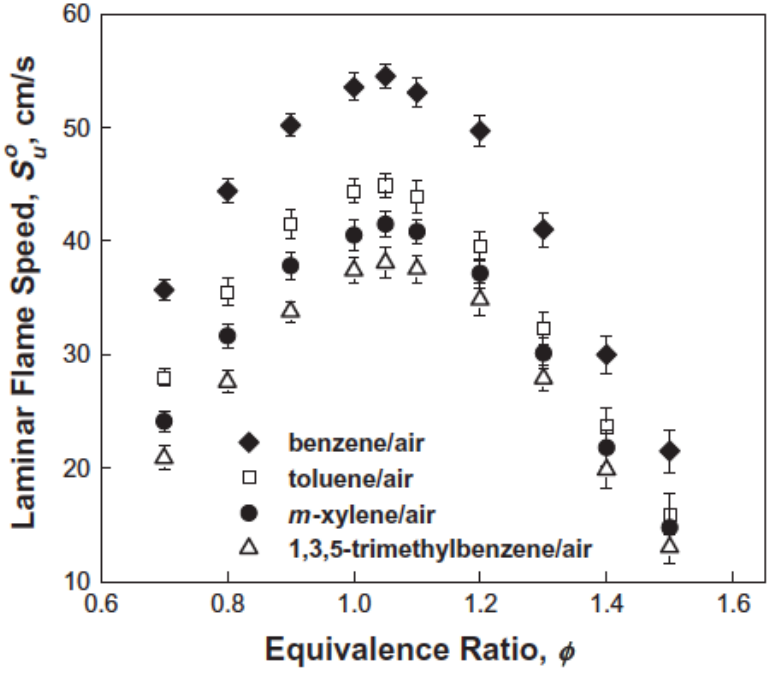


Fig. 5. Comparison of experimentally determined laminar flame speeds of benzene/air, toluene/air, *m*-xylene/air, and 1,3,5-trimethylbenzene/air mixtures at $T_u = 353$ K and $p = 1$ atm. The error bars represent 2σ uncertainty.

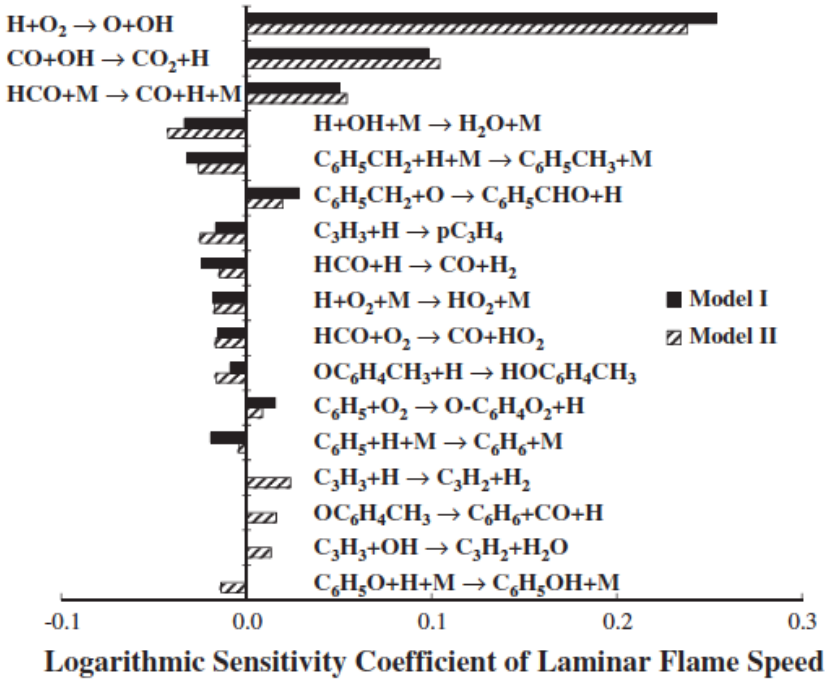
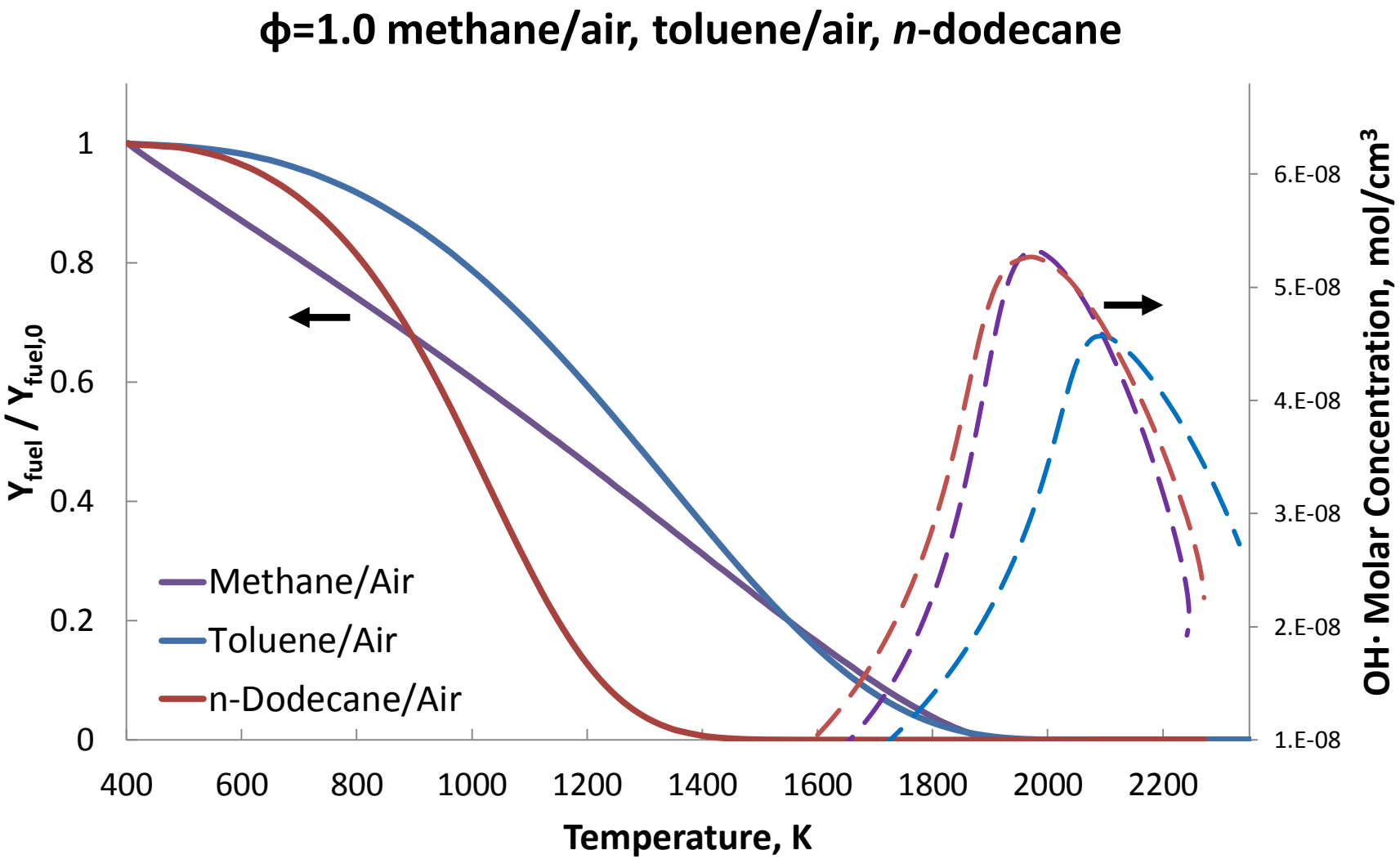


Fig. 8. Ranked logarithmic sensitivity coefficients of laminar flame speed with respect to reaction rate coefficients computed with Model I and II for a $\varphi = 1.0$ toluene/air mixture at $T_u = 353$ K and $p = 1$ atm.

Specific Objectives – Phase II

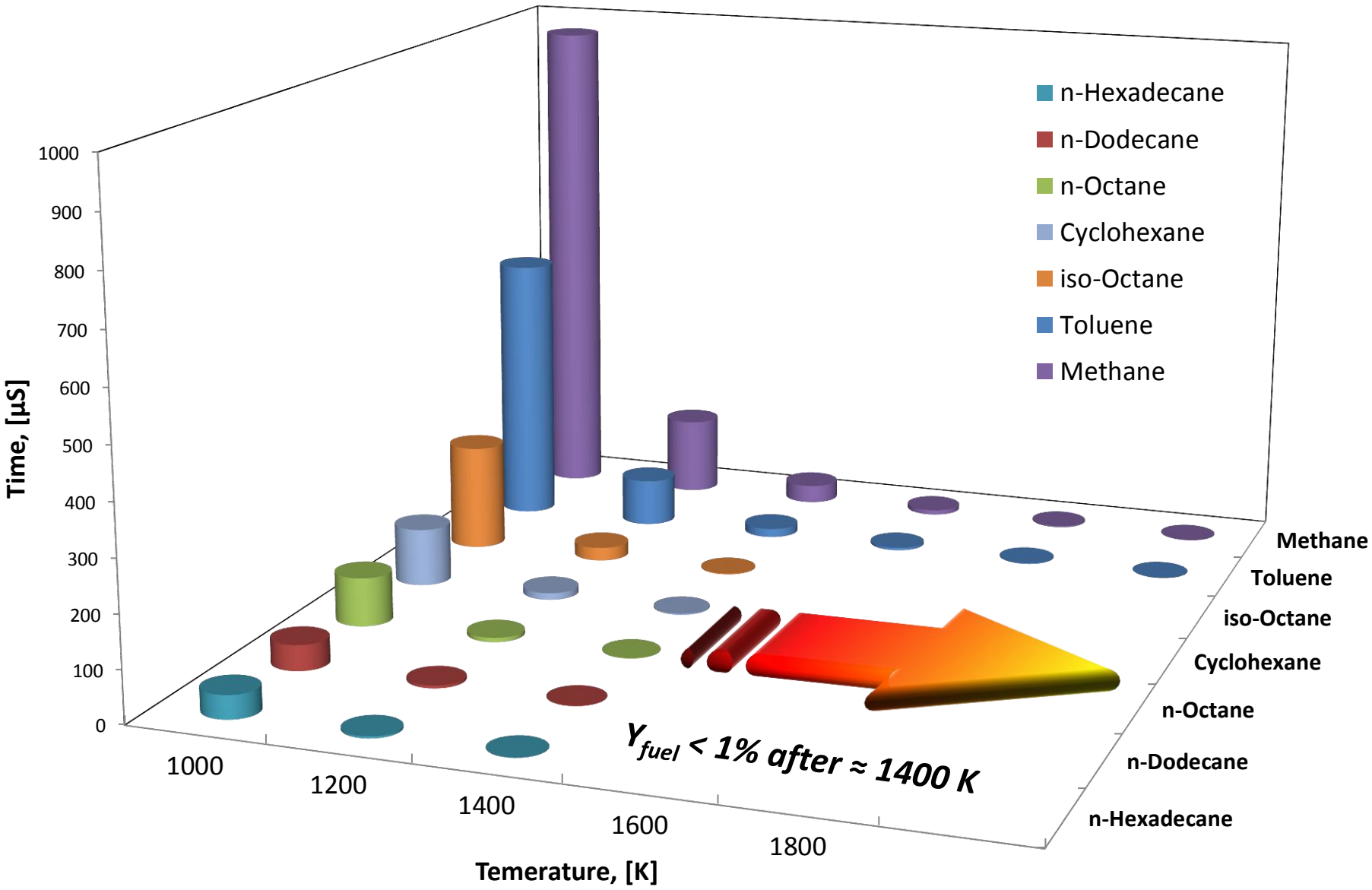
- **Use information obtained in Phase I to probe the details of fuel pyrolysis and oxidation in flame environments under a variety of conditions.**
- **Quantify experimentally tractable characteristics of highly turbulent jet flames for heavy fuels of relevance to air-breathing propulsion.**
- **Assess adequacy of existing knowledge obtained in turbulent flames using small MW fuels.**
- **Characterize probable heating time histories of fuels and identify the relevant rate-controlling kinetic steps.**
- **Assess whether kinetic model validation for surrogate fuels under "standard" laboratory conditions is sufficient.**
- **Develop new experimental approaches that would allow for measuring fundamental flame properties of relevance to highly turbulent flames and provide thus additional validation targets for the JetSurf 2.5 kinetic model.**
- **Add to existing turbulent flame knowledge by considering observables derived from low and large MW fuel experiments.**

Laminar Flame Structure

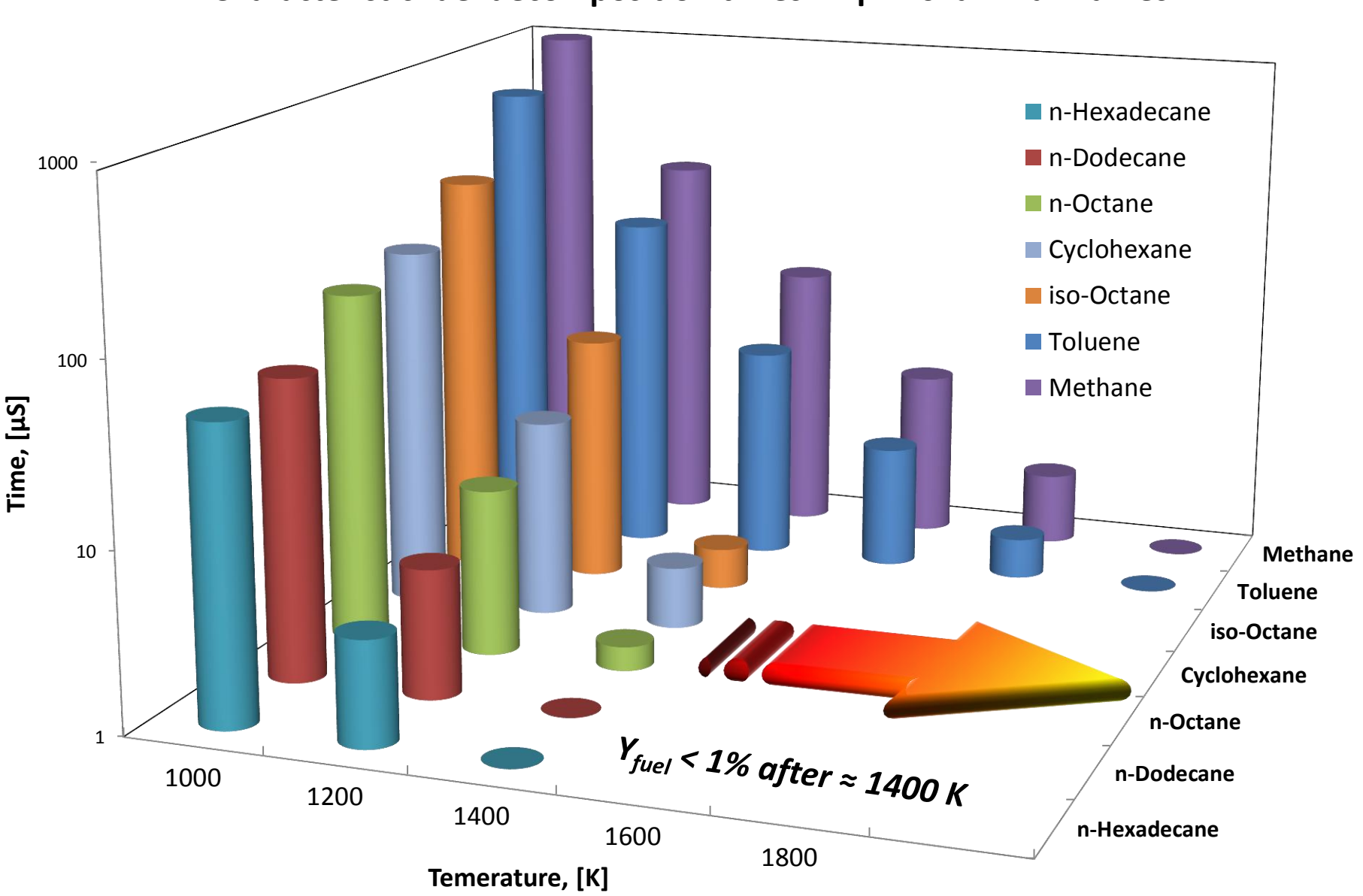


Fuel Decomposition (1)

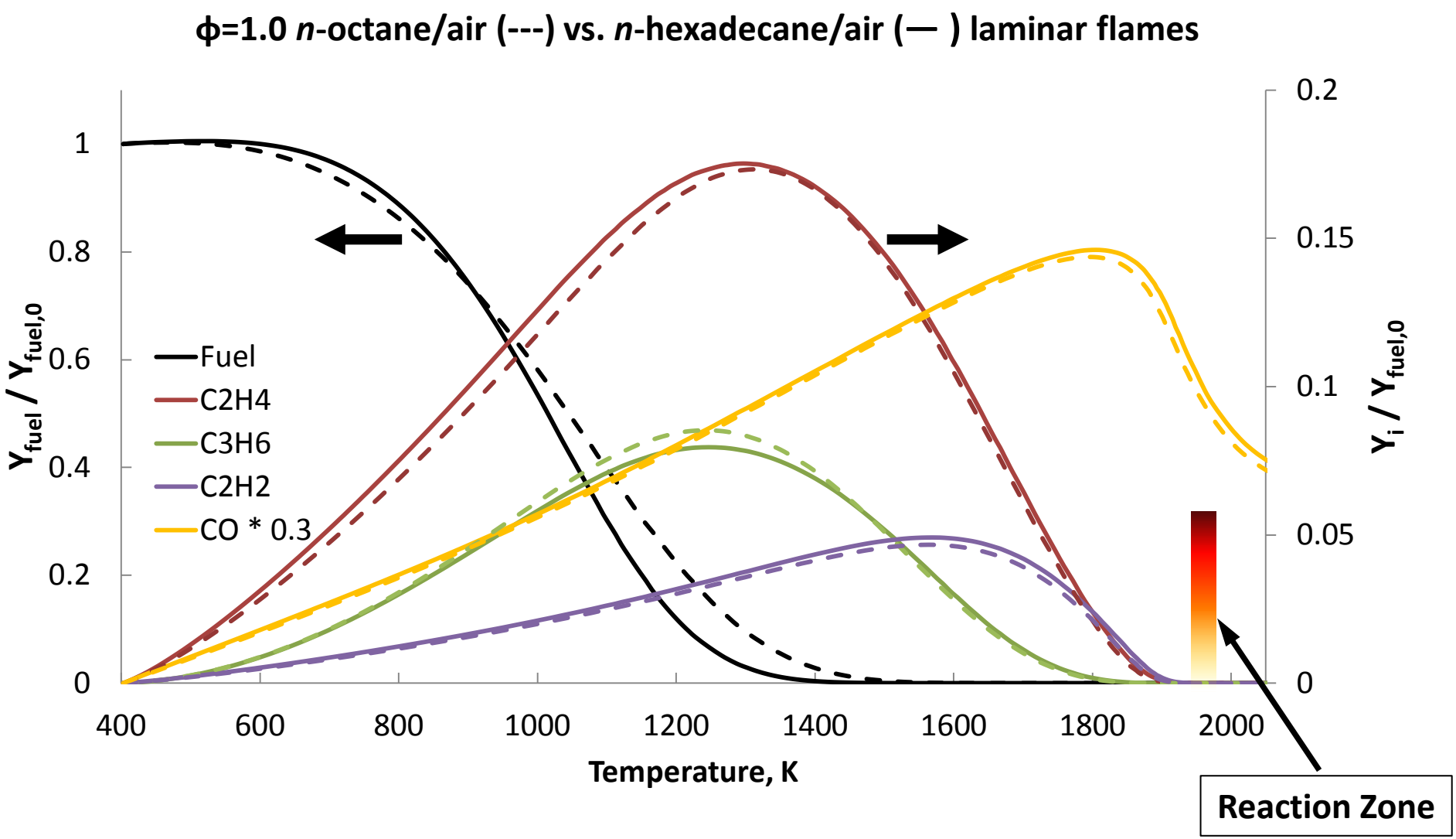
Characteristic fuel decomposition times in ϕ=1.0 laminar flames



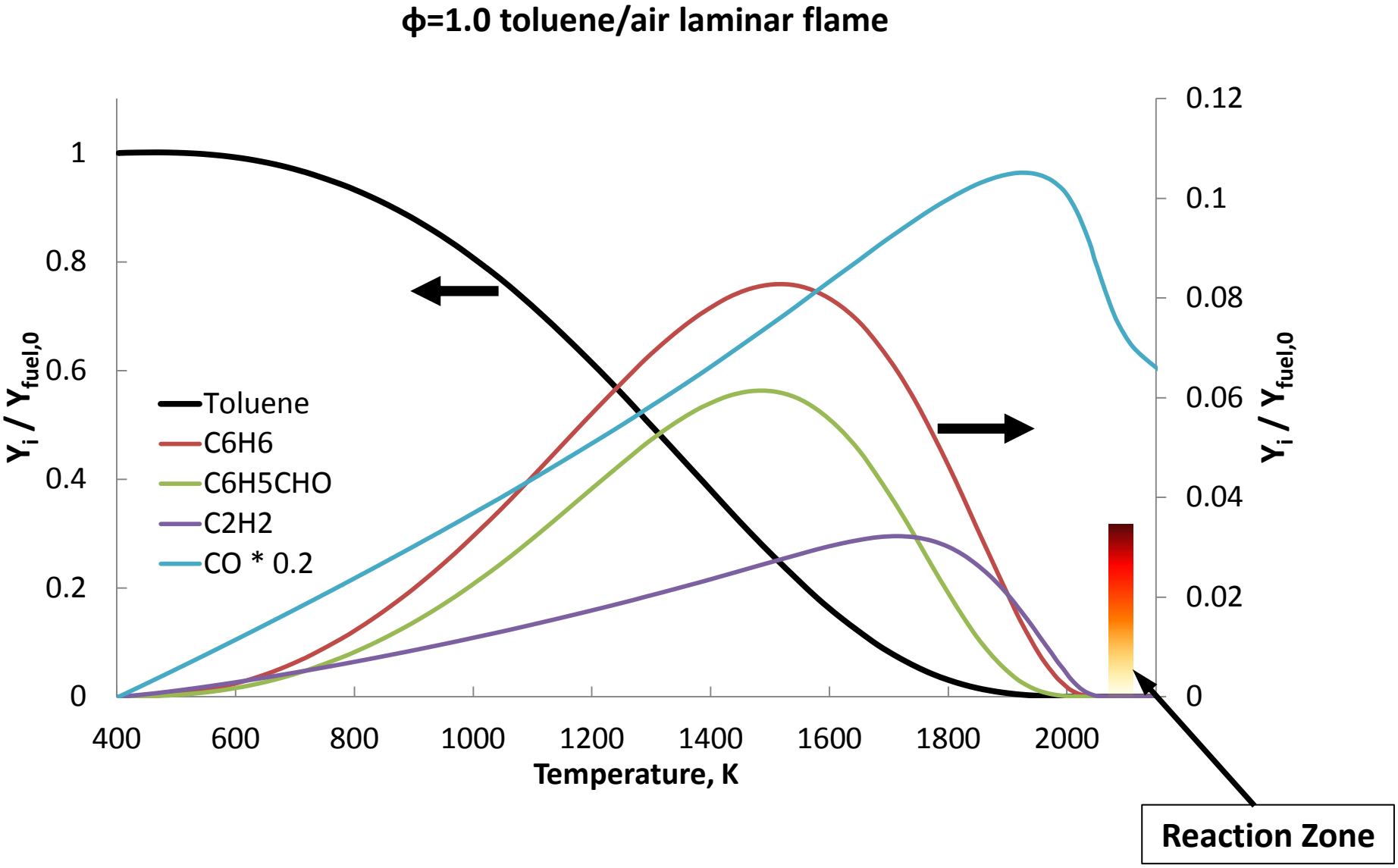
Fuel Decomposition (2)



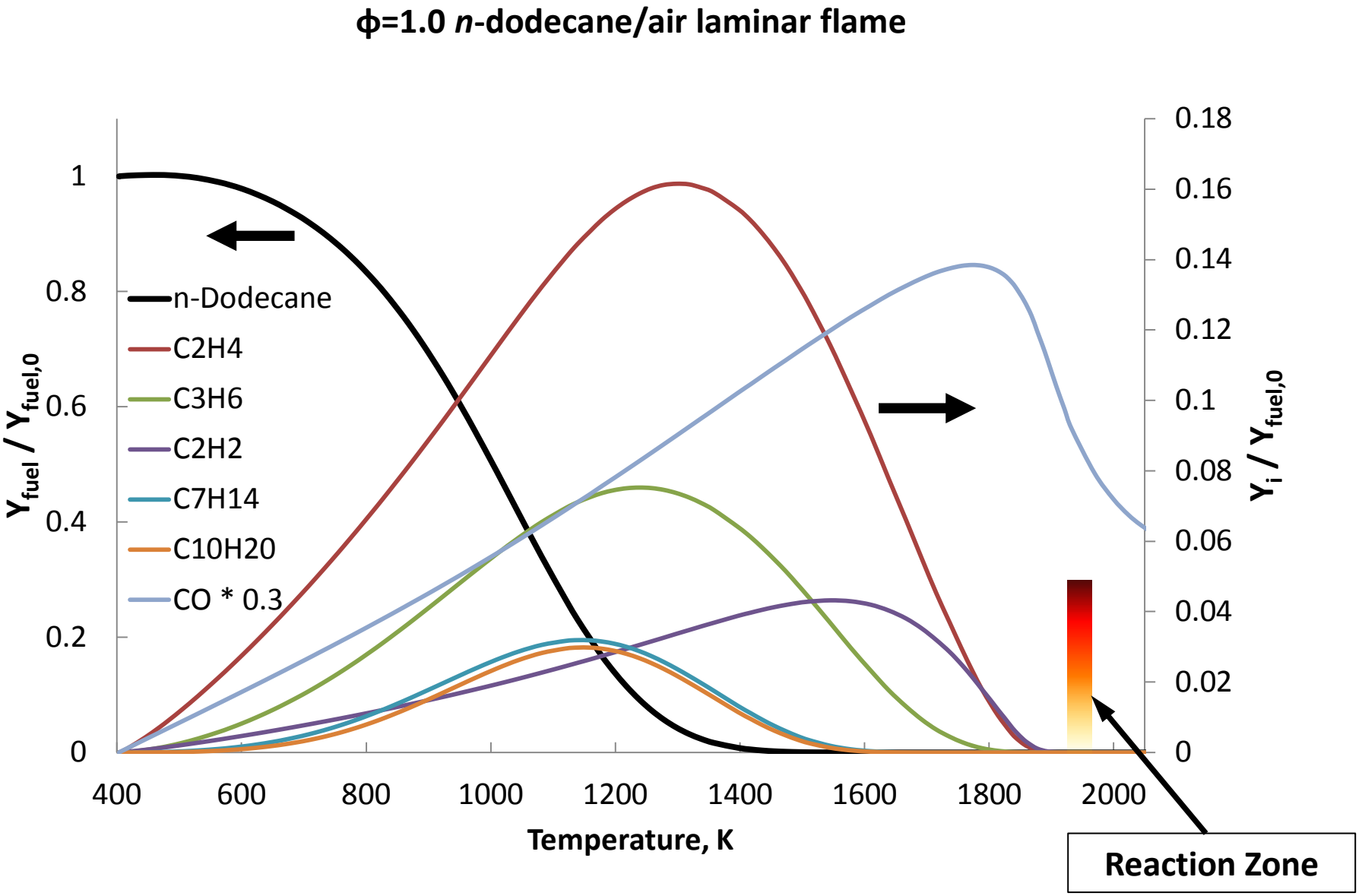
Major Intermediates – *n*-Alkanes



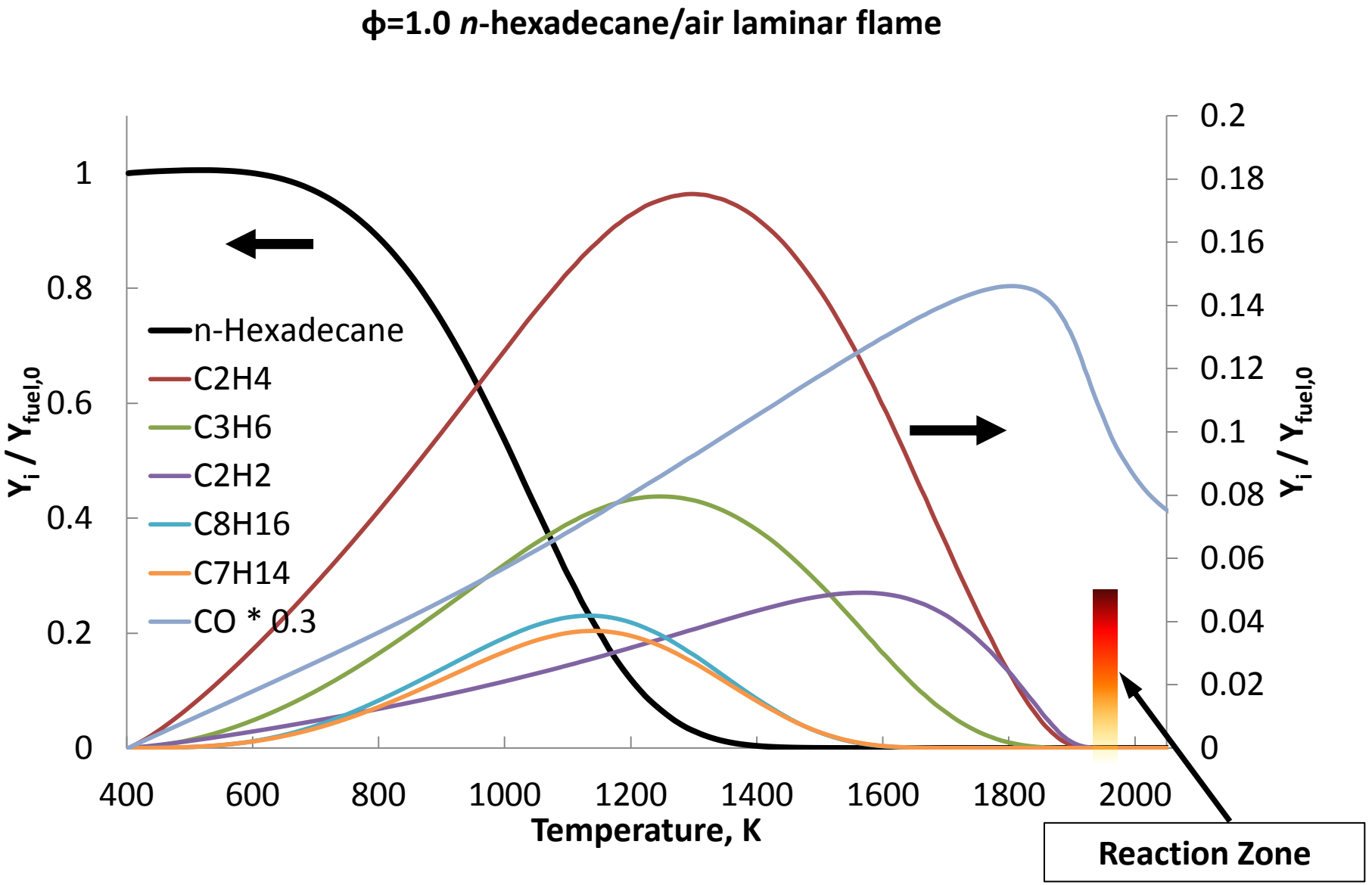
Major Intermediates - Toluene



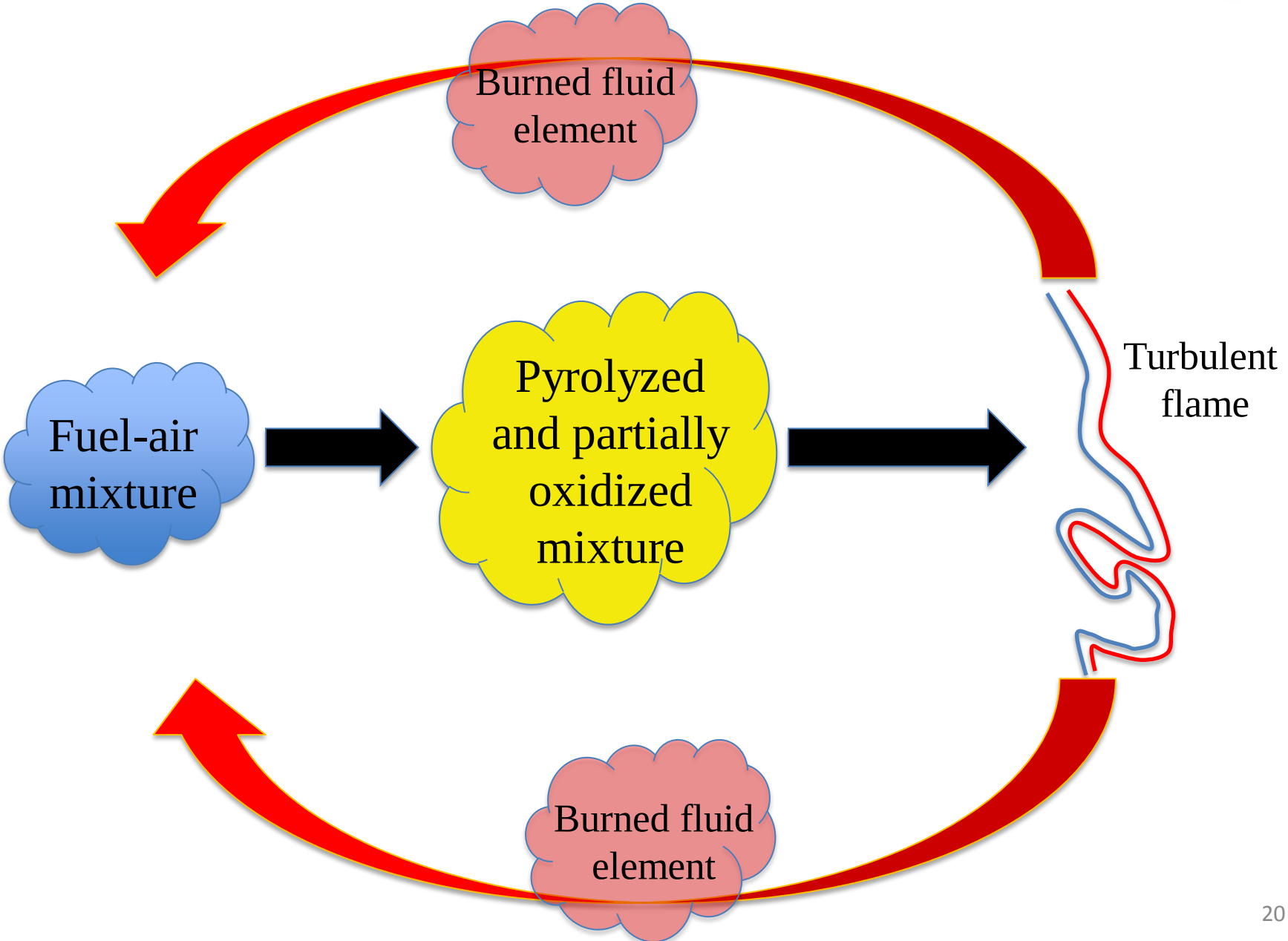
Major Intermediates – *n*-Dodecane



Major Intermediates – *n*-Hexadecane



“Free-Stream” Effects



"Sydney" Turbulent Flames

- **Bilger and coworkers have introduced the piloted premixed jet burner (PPJB) to study the effect of finite-chemistry effects in turbulent combustion.**
- **Main features:**
  - **A 4-mm diameter central jet (ϕ=0.5 CH_4/air or NG/air, U_o=50, 100, 150, 250 m/s, 2-3 kW).**
  - **A 23.5-mm OD / 4.5-mm ID disc surrounding the central jet to act as a pilot (ϕ=1.0 CH_4/air or NG/air, U_o=0.7 m/s, ~1 kW).**
  - **A 197-mm OD disk to provide co-flow of hot gases (ϕ=0.43 H_2/air, T_{ad}=1500 K, U_o=0.8 m/s, ~41 kW).**
- **Various stability regimes were identified:**

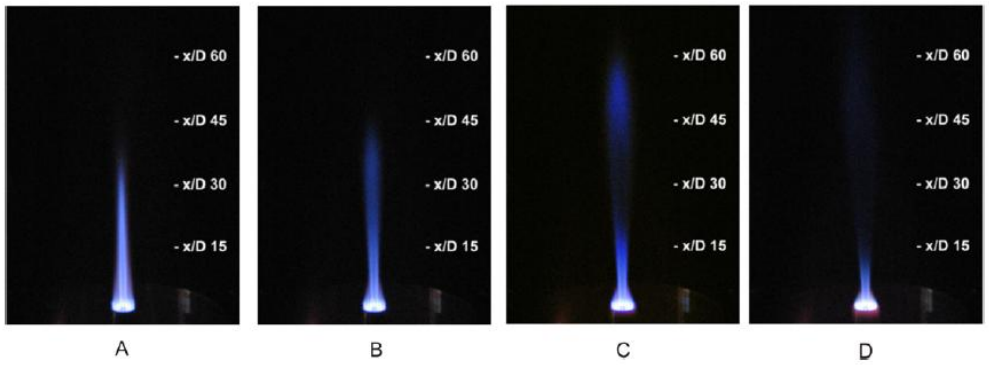
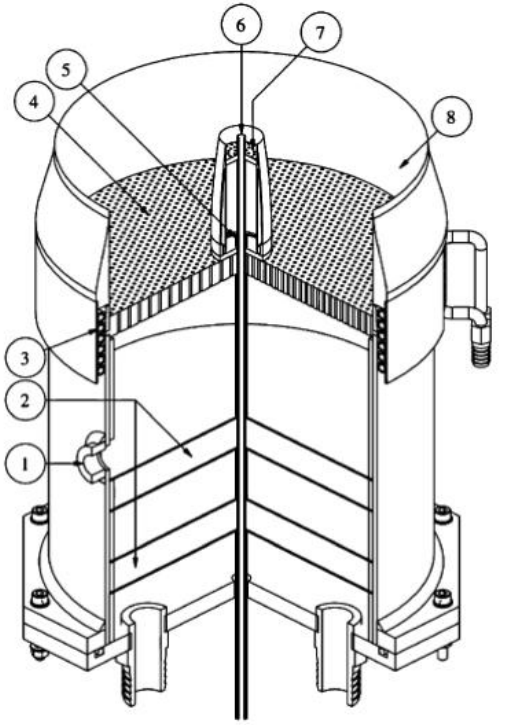
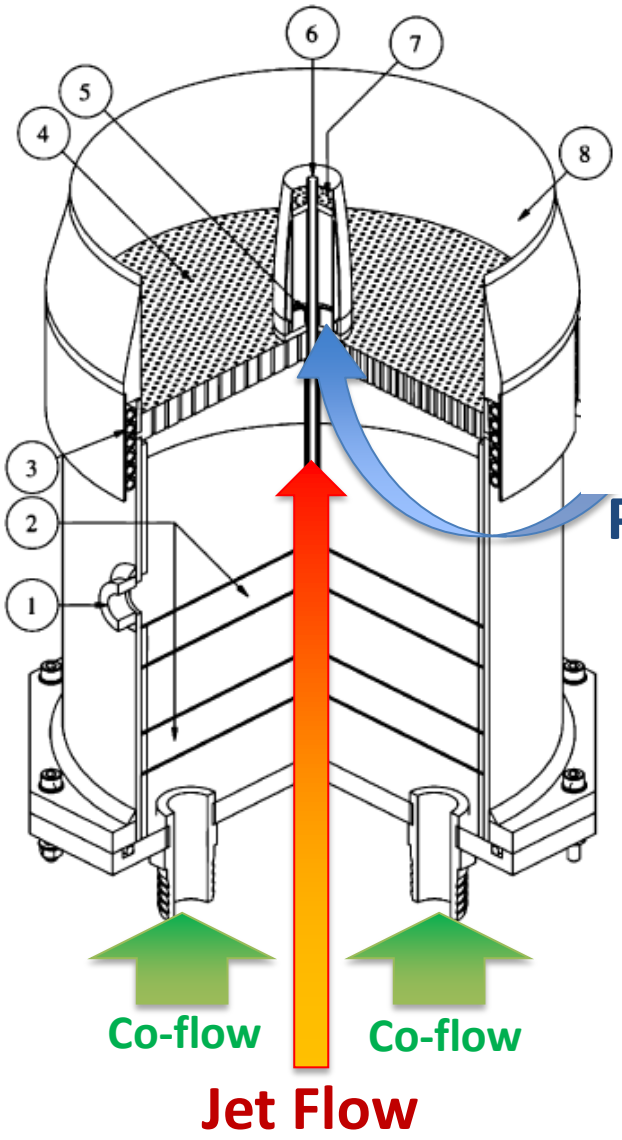


Fig. 3. Time-averaged images taken with a conventional color digital camera of the selected flames: (A) PM1-50, (B) PM1-100, (C) PM1-150, (D) PM1-200. Note: A, B, C, and D correspond to the respective regimes in Fig. 2.



Balloon number	Description
1	Flashback over-pressure sensing port
2	Glass bead filled cavities
3	Cooling water coil
4	Coflow perforated baseplate
5	Pilot mixture feed exit
6	Central jet exit
7	Pilot perforated baseplate
8	Coflow collar

"USC" Turbulent Flames

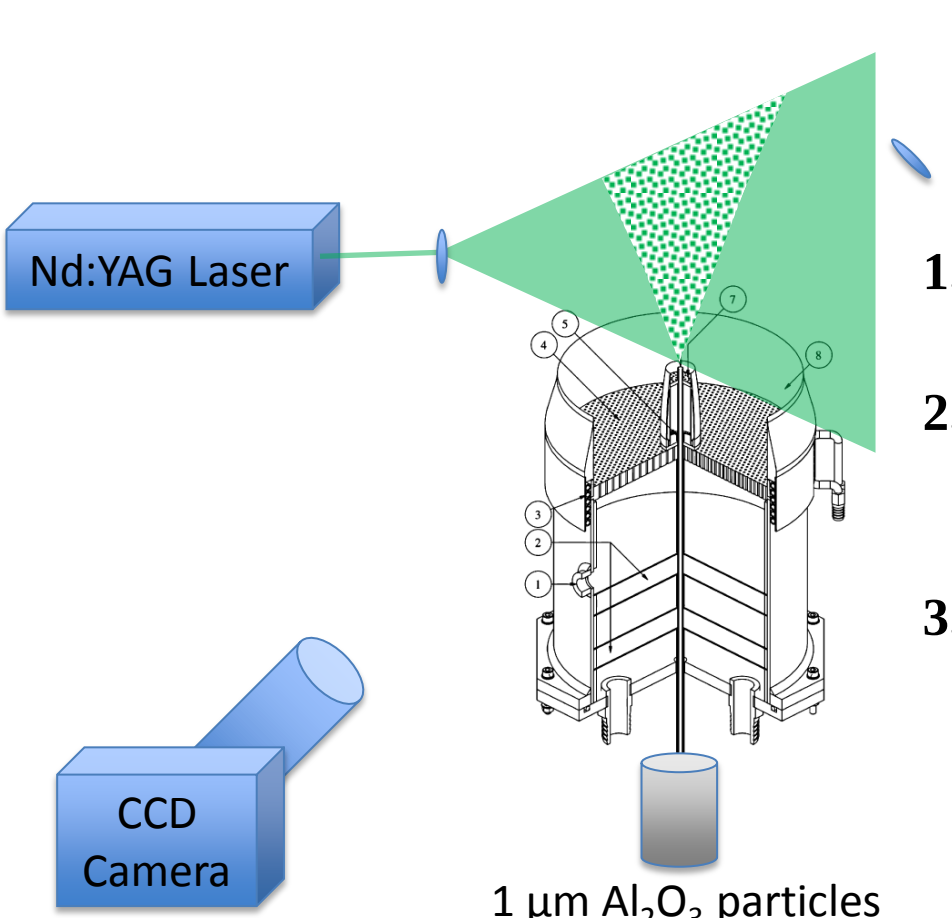


Jet Premixed Flame stabilized with a Pilot Flame

1. Central jet velocity ~ 100 m/s
2. Pilot flame velocity ~ 1 m/s
3. Co-flow was not used

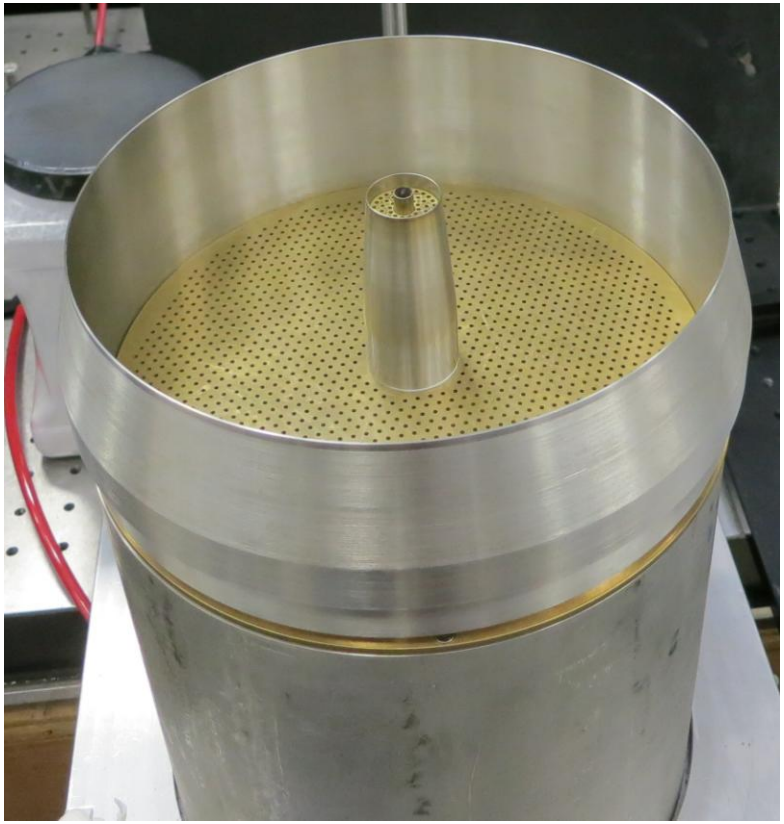
Volumetric flow rates finely controlled with sonic nozzles (mass flow meters for C_4 fuels)

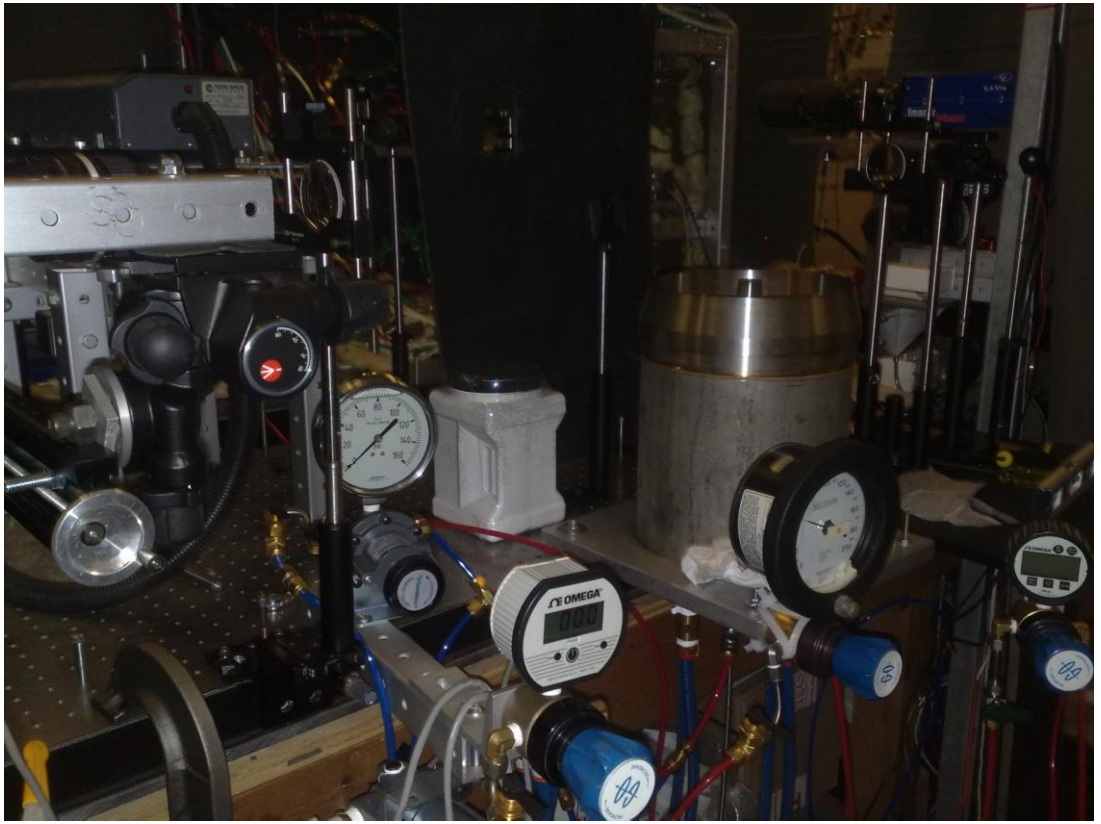
Optical Diagnostics



1. **Flame luminosity**
   (Limit: exposure time ~ 1 ms)
2. **Shadowgraph visualization of the flame**
   (Limit: imaged area size)
3. **Particle image velocimetry**
   (Limits: sampling frequency 11 Hz, δt=500 ns)

Experimental Layout





- **Pending issues:**
  - **Upgrade air compressor (short term)**
  - **Installation of explosion-proof, high-capacity exhaust system (short term)**
  - **Acquiring high-speed (kHz) diagnostics, e.g. tomographic PIV, PLIF (near term)**
  - **Acquiring temperature measuring diagnostics (longer term)**

Preliminary Investigations

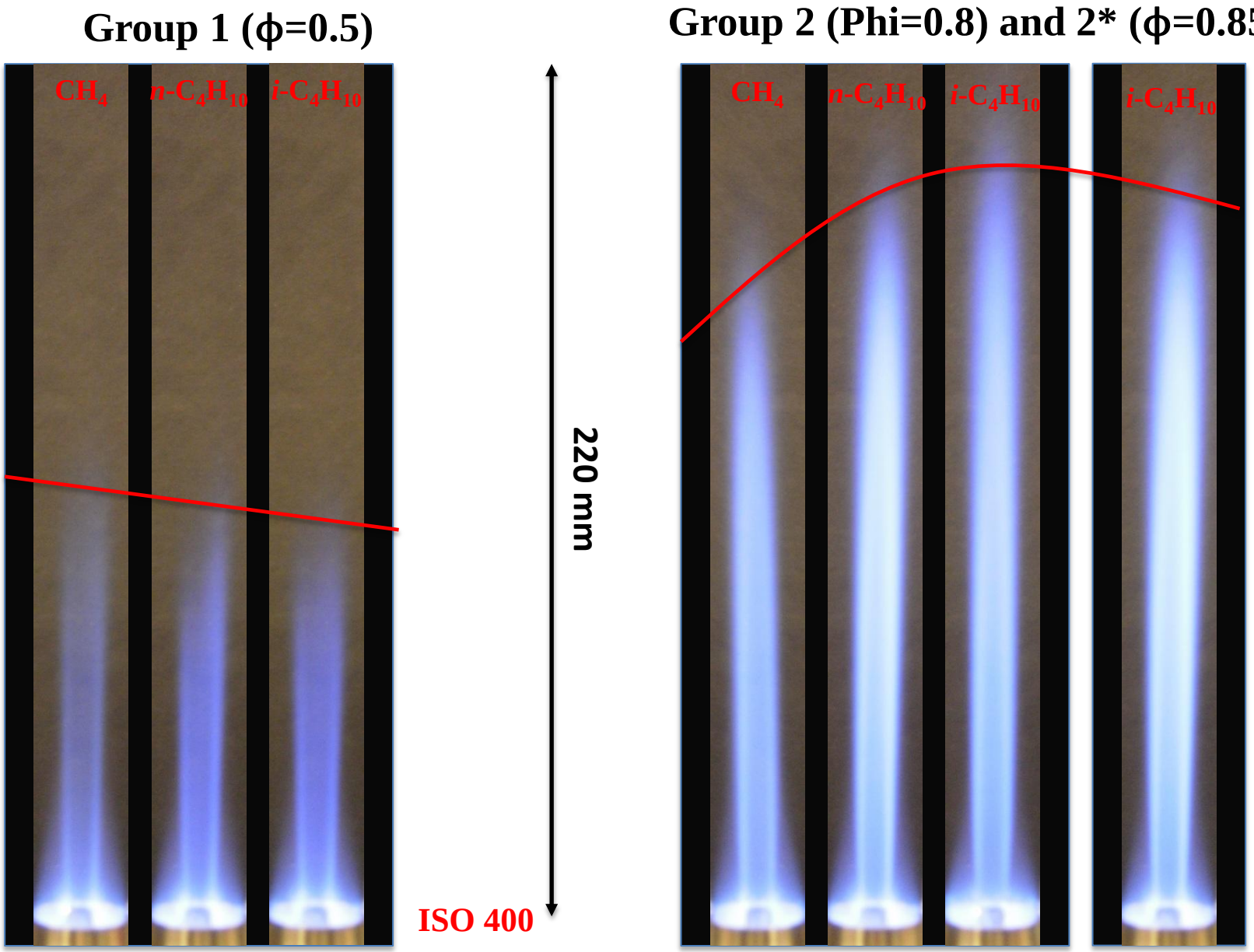
Pilot Flame	Fuel	CH_4
	ϕ	1
	T_{ad}, K	2224
	U_o, m/s	0.7
	Nozzle OD, mm	23.5
	Nozzle ID, mm	6.35

The characteristics of the pilot flame are the same in all experiments.

		Group 1			Group 2			Group 2*
		Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
Central Jet Flame	Fuel	CH_4	*n*-C_4H_{10}	*iso*-C_4H_{10}	CH_4	*n*-C_4H_{10}	*iso*-C_4H_{10}	*iso*-C_4H_{10}
	ϕ		0.5			0.8		0.85
	T_{ad}, K	1475	1503	1503	1995	2040	2040	2113
	S_u^o, cm/s	N/A	N/A	N/A	25.5 (26.9)	28.2 (30.8)	25.8 (24.9)	28.2 (27.5)
	U_o, m/s		34.2			34.2		34.2
	Nozzle ID, mm		5.84			5.84		5.84
	Re		12500			12500		12500

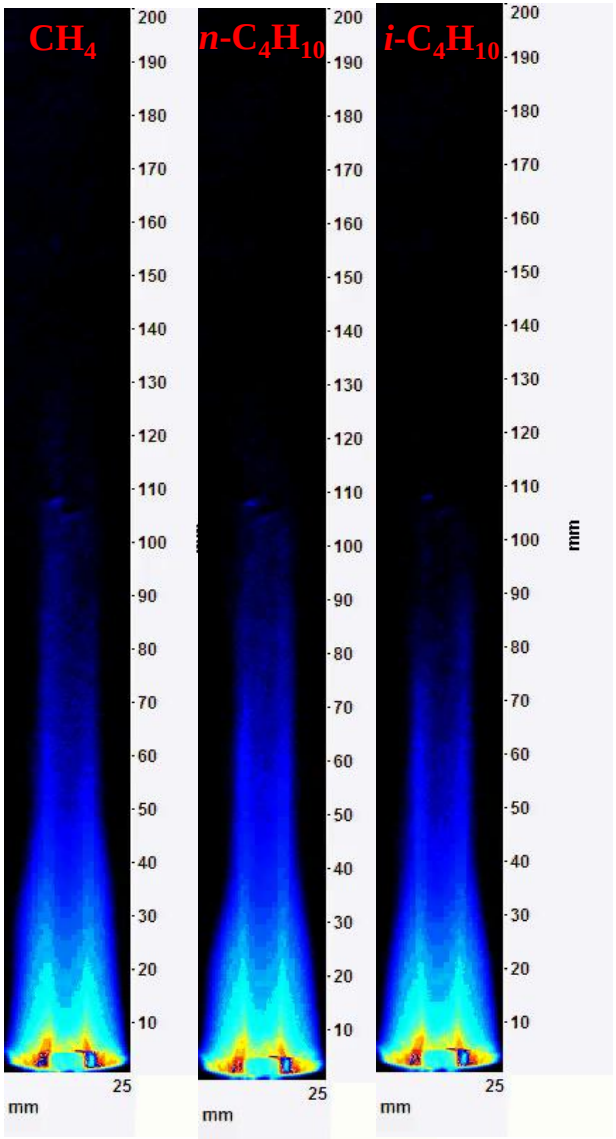
Variation of fuel (and oxidizer) will allow for assessing the role of fuel chemistry on the global and local behavior of turbulent flames.

Color Imaging with Standard Camera



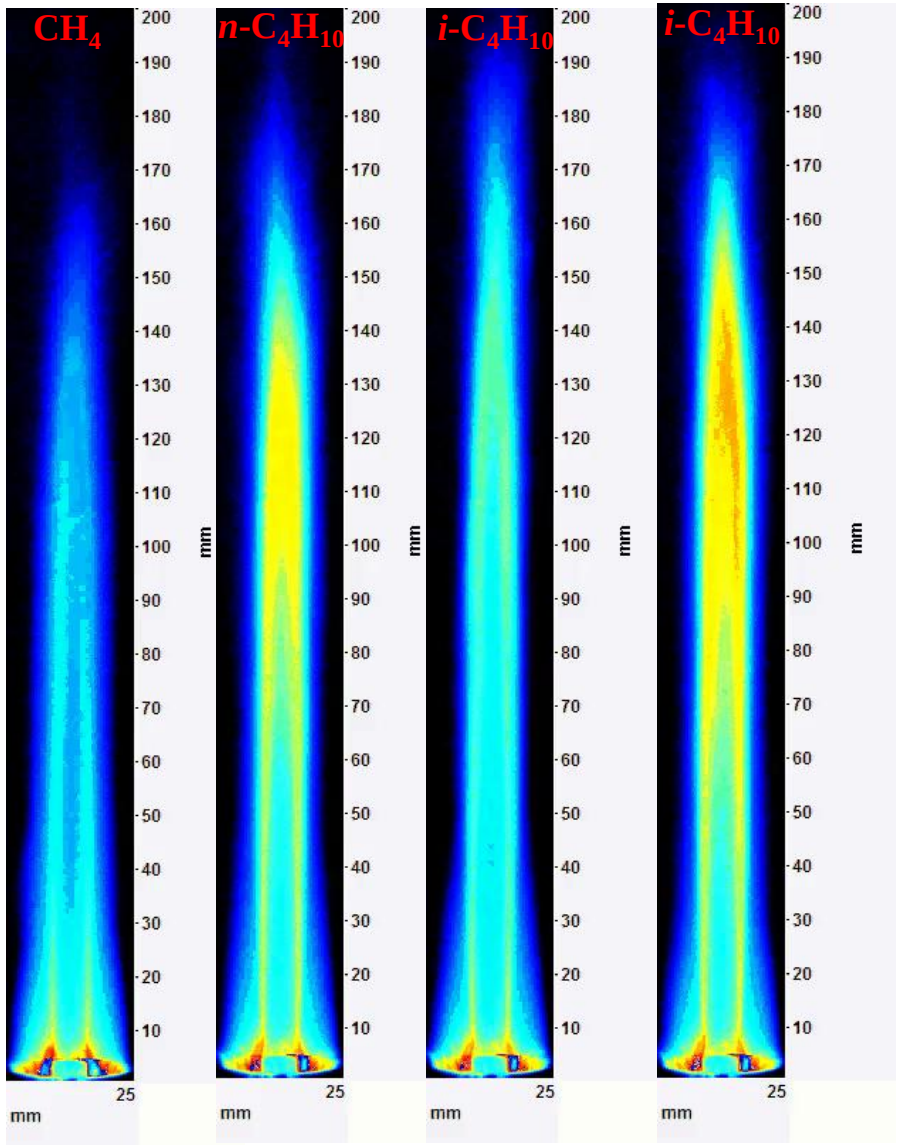
Flame Luminosity

Group 1 (ϕ=0.5)



200 mm

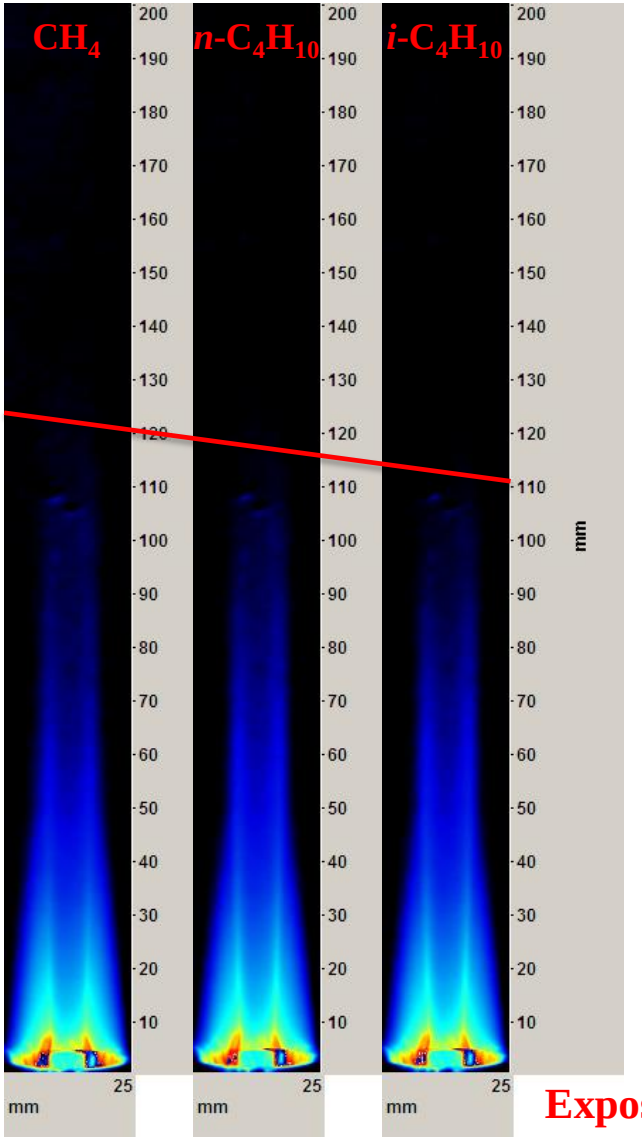
Group 2 (Phi=0.8) and 2* (ϕ=0.85)



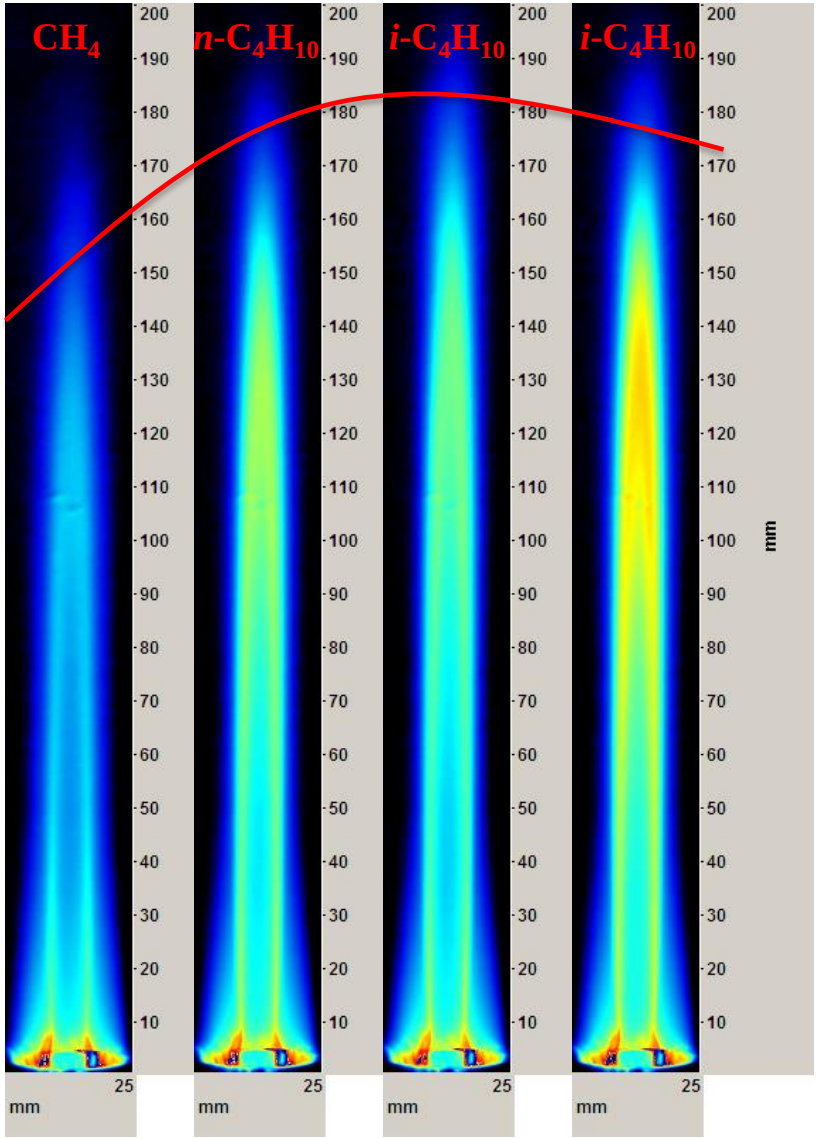
Exposure time 5 ms (not adequate for high temporal resolution)

Average Luminosity

Group 1 (ϕ=0.5)

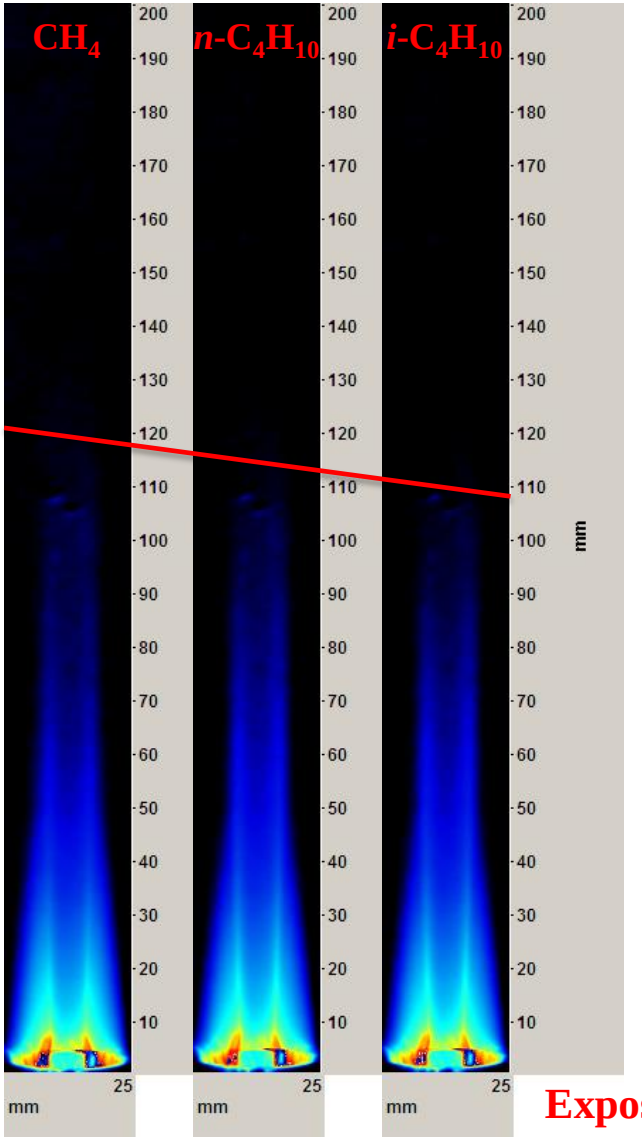


Group 2 (Phi=0.8) and 2* (ϕ=0.85)



Average Luminosity

Group 1 (ϕ=0.5)



For weakly-burning flames, flame length is affected by local quenching at the flame tip due to strain rate, reactant dilution, and/or heat loss. Observed differences could be attributed to:

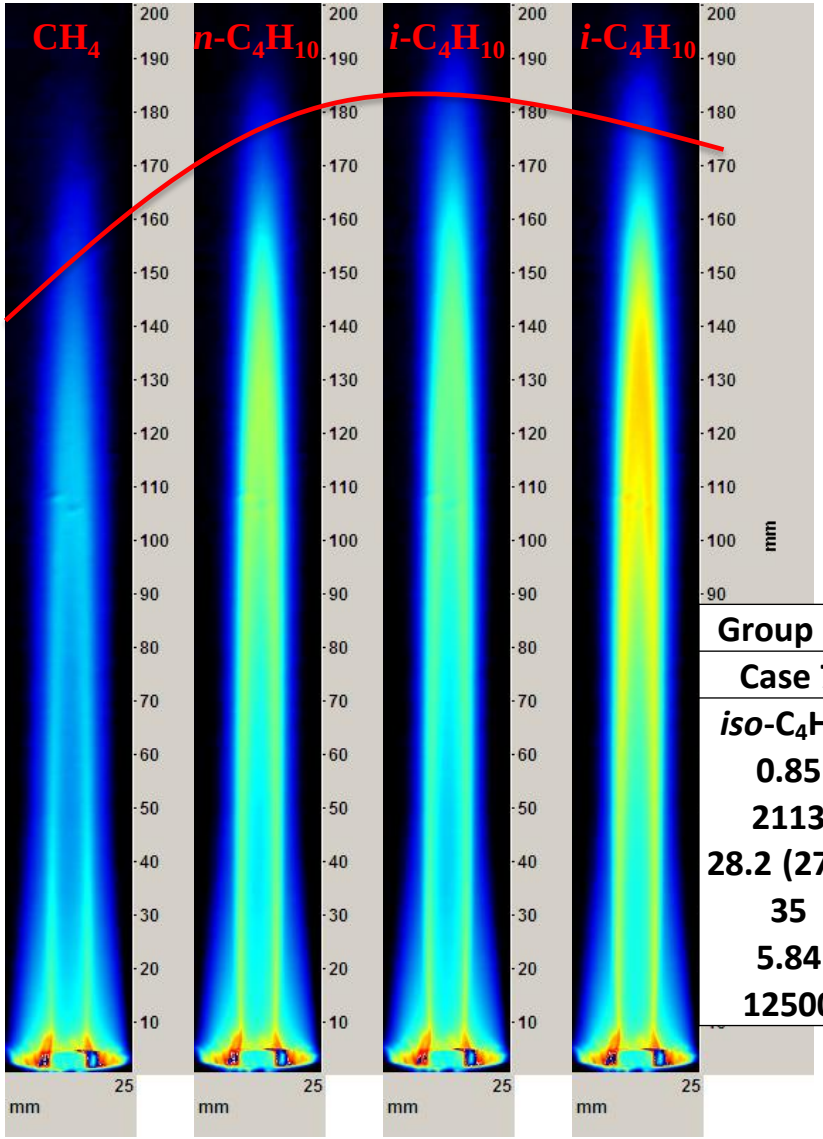
- Differences in reactivity
- Differences in fuel diffusivity

	Group 1		
	Case 1	Case 2	Case 3
Fuel	CH_4	*n*-C_4H_{10}	*iso*-C_4H_{10}
ϕ		0.5	
T_{ad}, K	1475	1503	1503
S_u^o, cm/s	N/A	N/A	N/A
U_o, m/s		35	
Nozzle ID, mm		5.84	
Re		12500	

Average Luminosity

Group 2 (Phi=0.8) and 2* (ϕ=0.85)

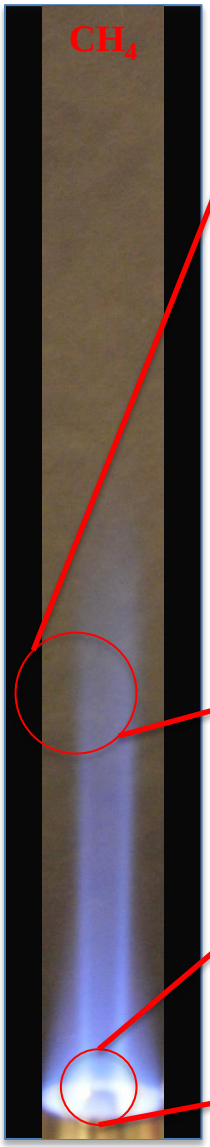
For strongly-burning flames, flame length appears to correlate well with mixture reactivity for fuels of similar MW. Comparisons for fuels with notably different MW's are more challenging.

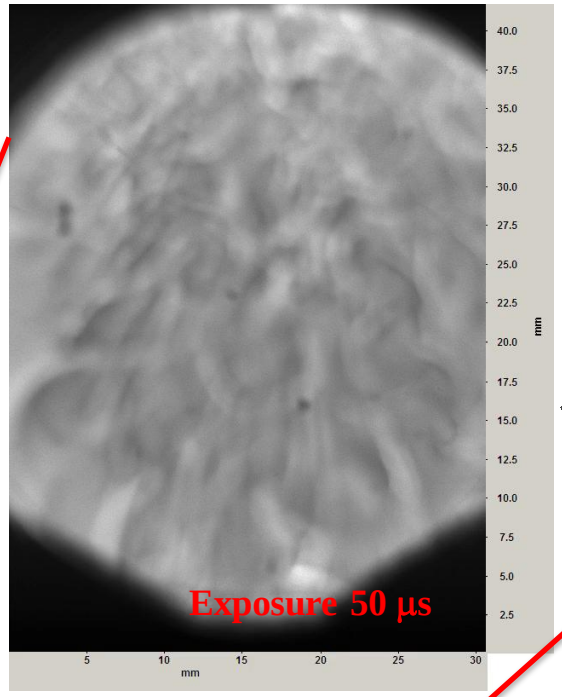


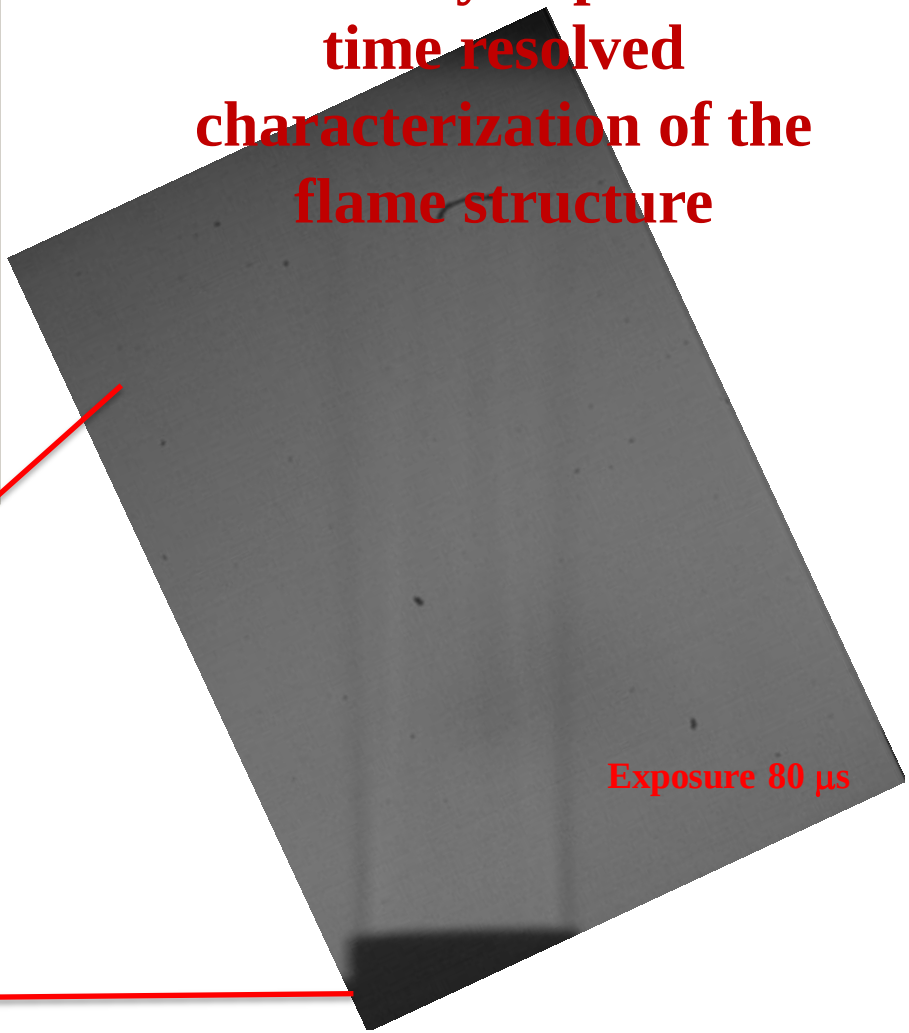
	Group 2			Group 2*
	Case 4	Case 5	Case 6	Case 7
Fuel	CH_4	*n*-C_4H_{10}	*iso*-C_4H_{10}	*iso*-C_4H_{10}
ϕ	0.8			0.85
T_{ad}, K	1995	2040	2040	2113
S_u^o, cm/s	25.5 (26.9)	28.2 (30.8)	25.8 (24.9)	28.2 (27.5)
U_o, m/s	35			35
Nozzle ID, mm	5.84			5.84
Re	12500			12500

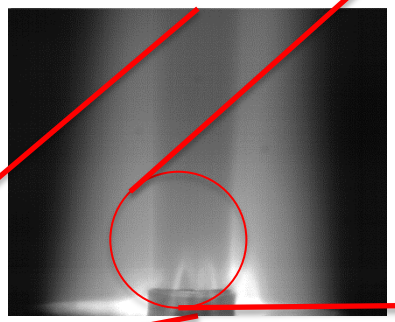
Exposure 5 ms

Shadowgraph images





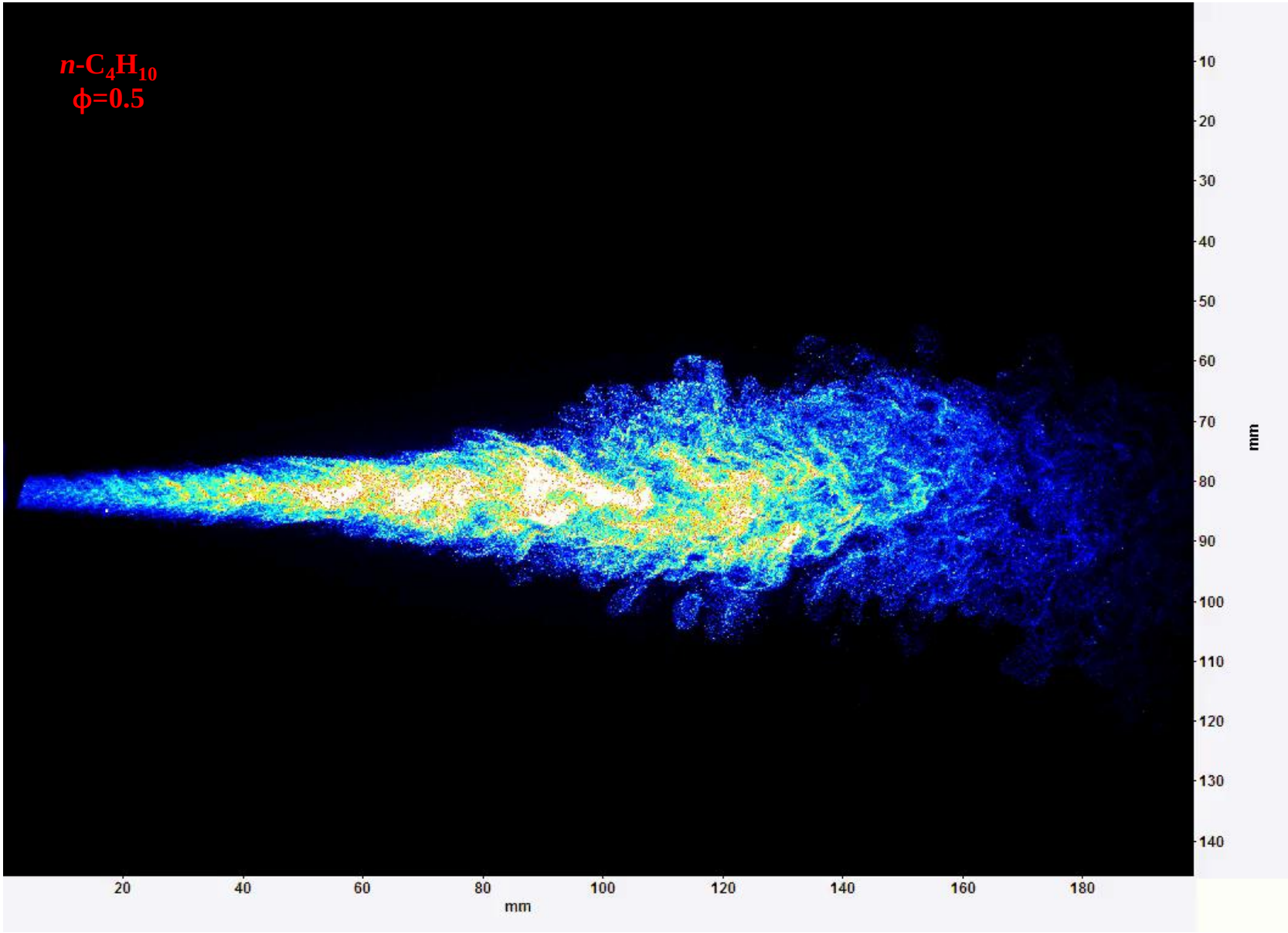




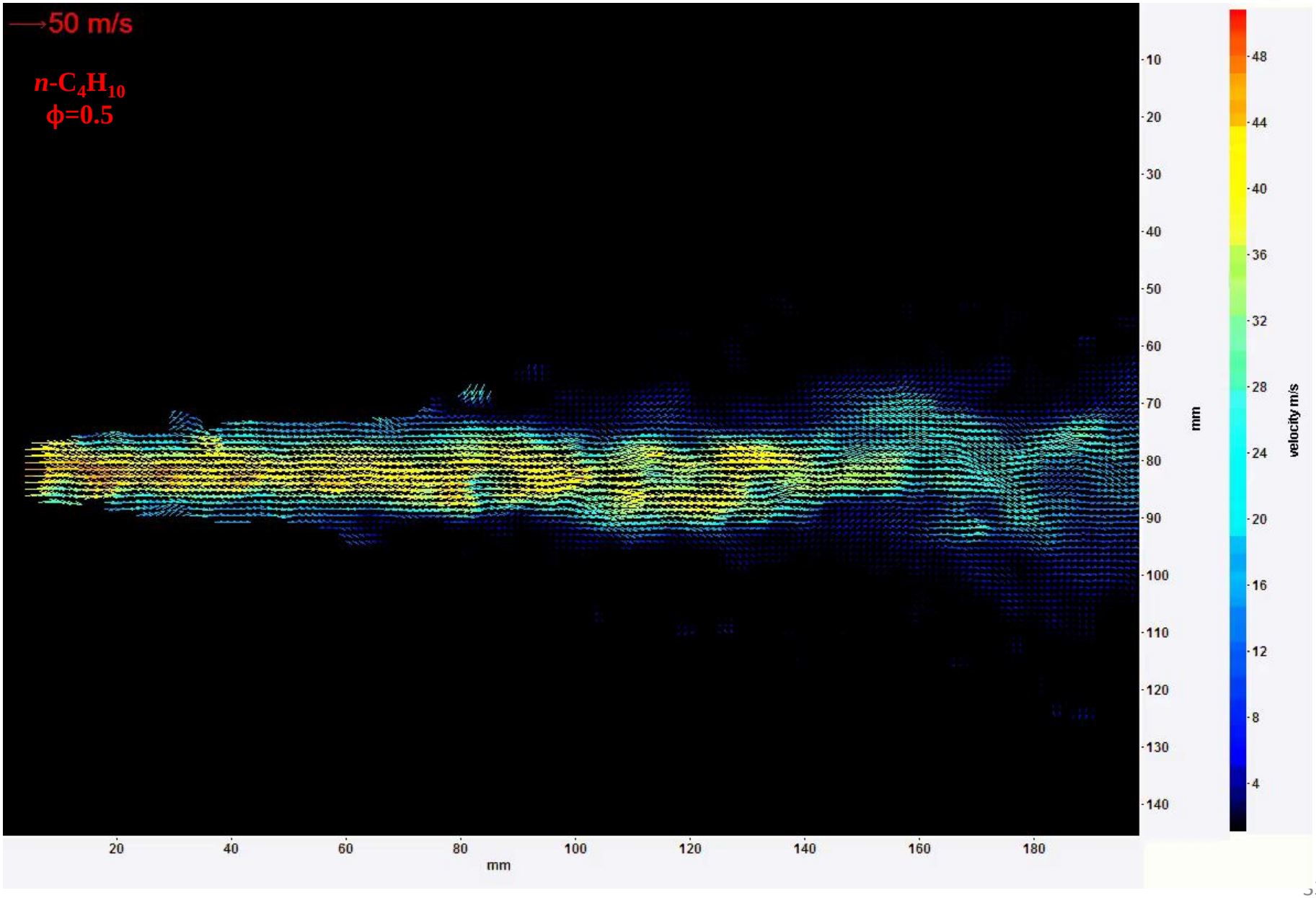
Exposure 50 ms

Possibility to perform time resolved characterization of the flame structure

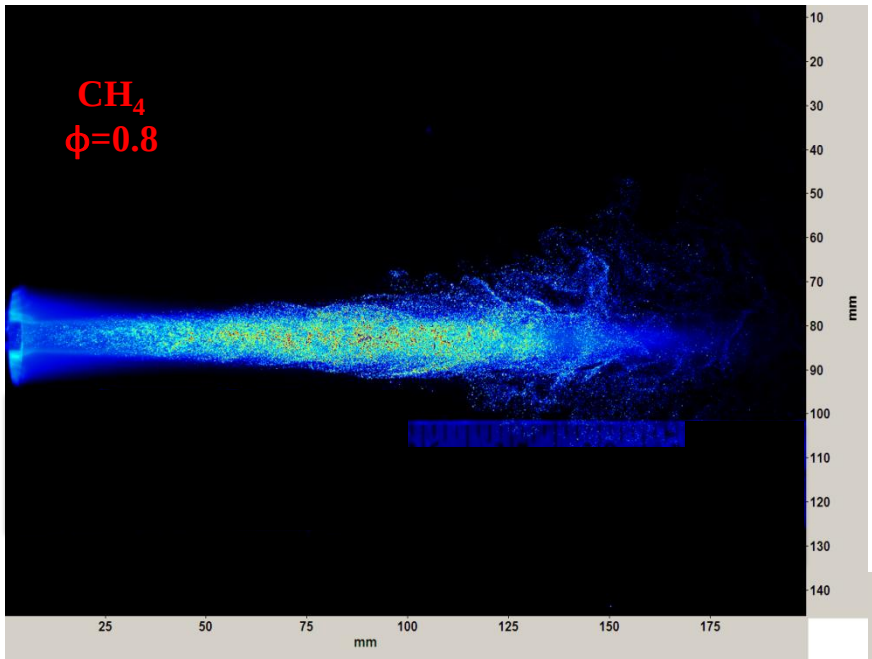
Particle Image Velocimetry

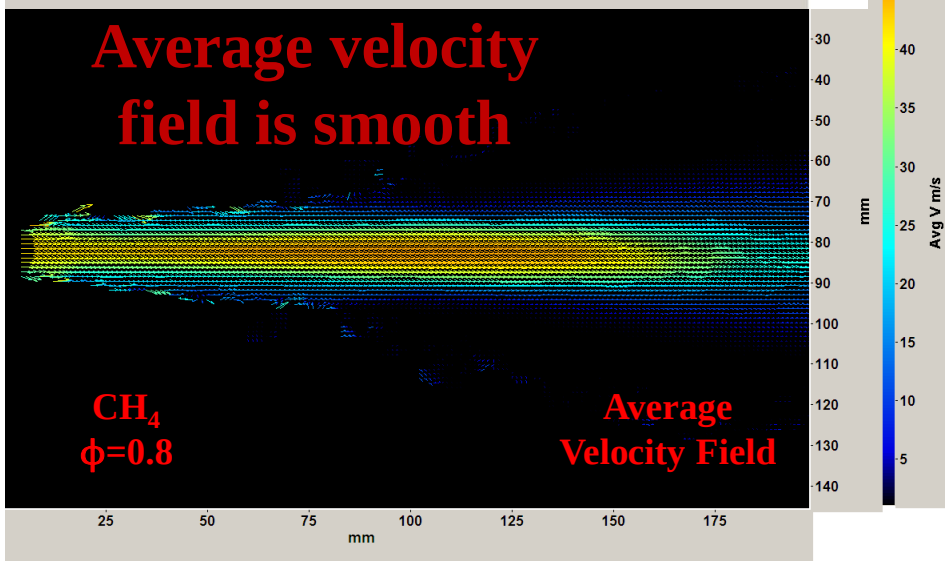


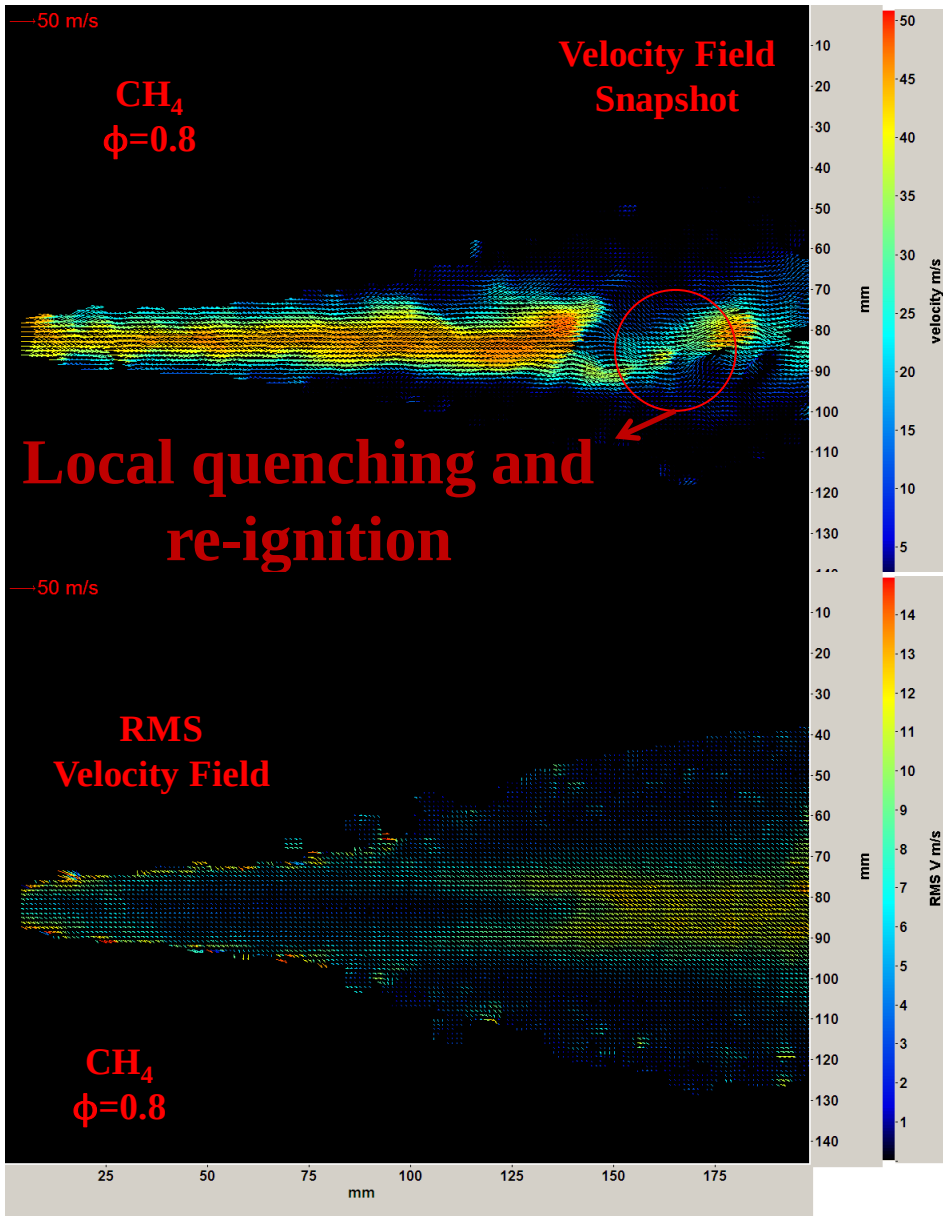
Particle Image Velocimetry



Velocity field

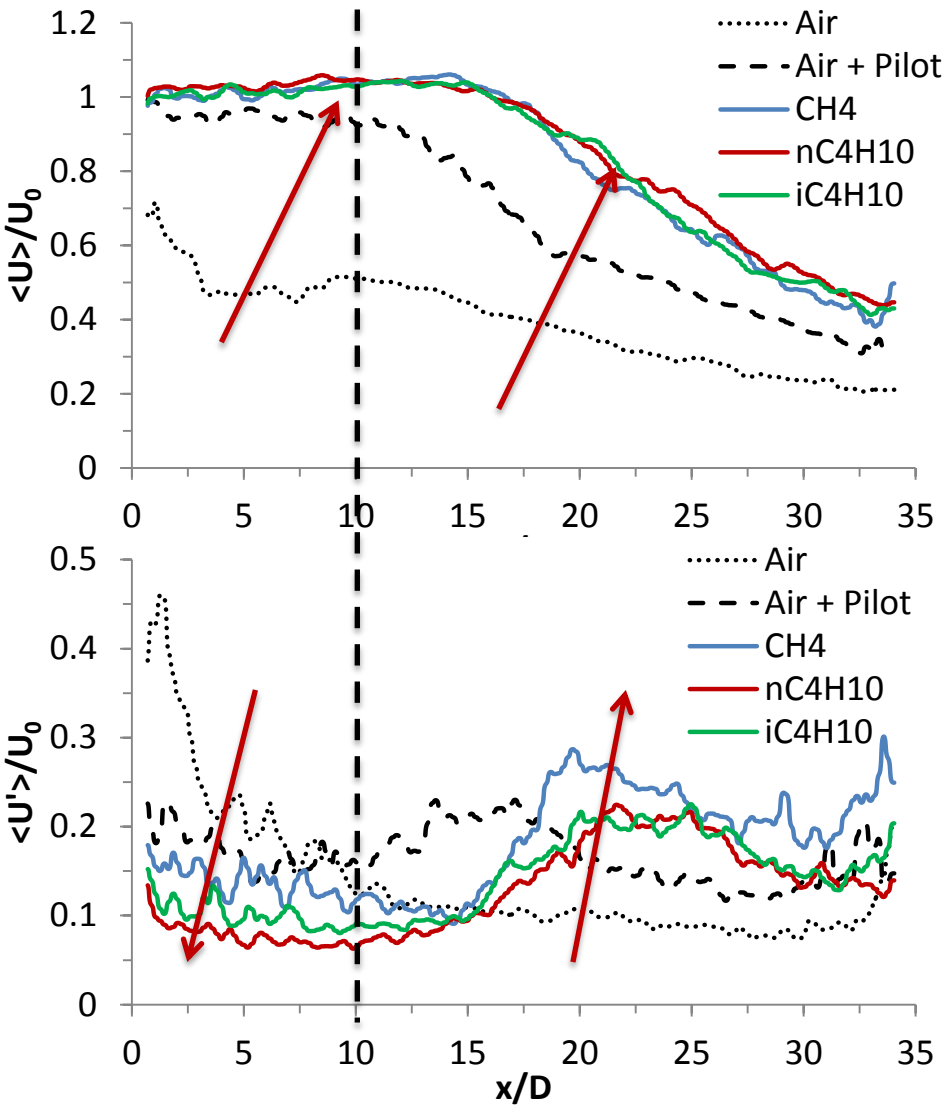






Average Velocities – Group 1

Profiles at R=0



The presence of the pilot and subsequently of the flame tends to:

- **increase the mean velocity**
- **decrease the turbulence intensity at small x/Ds**
- **increase the turbulence intensity at large x/Ds**

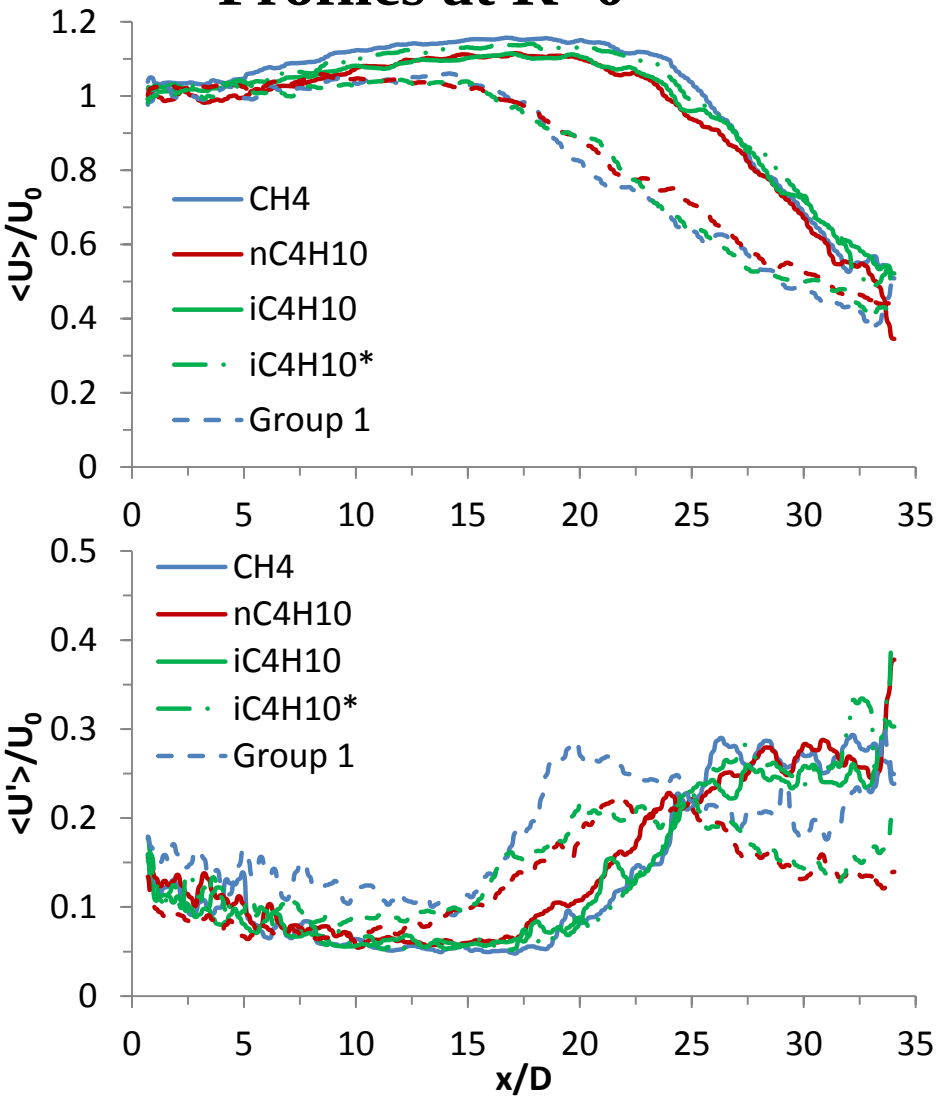
Results in qualitative agreement with the Sydney results obtained though in the presence of the co-flow.

Fuel effects:

- **negligible on the mean velocity**
- **notable on turbulence intensity**

Average Velocities – Groups 1 & 2

Profiles at R=0



Mean velocity:

- increases with overall reactivity
- does not vary with the fuel types considered

Turbulence intensity:

- decreases as overall reactivity increases at small x/Ds
- Starts increasing as overall reactivity increases at large x/Ds

Summary and Future Work

- **Fundamental data on ignition, propagation, and extinction of laminar flames have been experimentally determined under "standard laboratory conditions" for all possible fuel chemical classifications relevant to surrogate jet fuel formulations. Data have been key validation targets for the JetSurf 2.0 kinetic model.**
- **Analysis of laminar flame structures using the JetSurf 2.0 kinetic model showed that with the exception of aromatics, large MW hydrocarbons do decompose readily before the main oxidation zone, which can impact the surrogate fuel development approach.**
- **Interactions between unburned and burned fluid elements in a turbulent flame environment could decompose the fuel in the "free-stream." Under such conditions, a multi-component mixture is fed into the flame and the definitions of various mixture properties including Le number and laminar flame speed become challenging.**
- **Preliminary results on piloted turbulent jet flames suggest that the choice of fuel could have an effect on both the global flame behavior and its local structure. Fluid dynamics results in qualitative agreement with those of Bilger and co-workers.**
- **The turbulent jet flame studies will be intensified and a variety of fuels and oxidizers will be investigated to isolate further the role of fuel kinetics on turbulent combustion.**
- **New experiments will be developed to measure fundamental flame properties appropriate for the validation of the JetSurf 2.5 kinetic model.**